

# MODELLING THE FATE OF AIR POLLUTANTS EMITTED FROM A TIME DEPENDENT POINT SOURCE : EFFECTS OF REMOVAL MECHANISMS

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for the Degree of*  
**DOCTOR OF PHILOSOPHY**

*By*  
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*to the*  
**DEPARTMENT OF MATHEMATICS  
INDIAN INSTITUTE OF TECHNOLOGY KANPUR**  
JUNE, 1992

*To,*  
*My Mother Smt. Shanti Devi*  
*and*  
*Father Shri S. M. Tripathi*  
*With Profound Respect.*

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## CERTIFICATE

This is to certify that the matter embodied in the thesis entitled "MODELLING THE FATE OF AIR POLLUTANTS EMITTED FROM A TIME DEPENDENT POINT SOURCE : EFFECTS OF REMOVAL MECHANISMS" by Mr. Ram Naresh for the award of Degree of Doctor of Philosophy of the Indian Institute of Technology Kanpur is a record of bonafide research work carried out by him under my supervision and guidance. The results embodied in this thesis have not been submitted to any other University or Institute for the award of any degree or diploma.



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June, 1992



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## CHAPTER I

### GENERAL INTRODUCTION

#### 1.0 INTRODUCTION

Modern civilization has become very complex with increasing demands of new and more resources in terms of materials, energy, habitats, etc. Rapid industrialization, fast population growth and associated pollution have created various kinds of problems leading to deterioration of our environment and ecology to a very undesirable level, lowering the carrying capacity of the earth to such an extent that if appropriate measures are not taken soon, the survival of the species will be threatened. Thus, conservation of resources, sustainable development and environmental protection by controlling the emission of pollutants are major socio-economic, scientific and technological challenges that our society faces today.

In this thesis, therefore, the problems related to the fate of air pollutants and their removal in the atmosphere are studied using mathematical models.

#### 1.1 AIR POLLUTION

The term environmental pollution may be defined as any undesirable addition to the environment which is harmful to man and his biosphere. In other words, it is the presence of undesirable contaminants in the environment in the form of gas, smoke, dust, fume, mist, waste disposal, etc. in such quantities and of such duration as to become injurious to human, plant and animal life, harmful to our living, to our enjoyment and to

historical monuments and other structures. Environmental pollution is generally divided into four broader classes : (i) Air Pollution (ii) Water Pollution (iii) Land/Soil Pollution, and (iv) Noise Pollution. The term social pollution is also sometimes used for abnormalities that arise in our society due to over population, crowding in habitats, rural migration, etc. Our main concern here is to study only certain aspects of air pollution using mathematical models.

#### 1.1.1 Air Pollutants

Various gases and particulate matters emitted in the atmosphere by industrial stacks, automobiles, energy generating units, cooking appliances, etc., in concentrations significantly higher than their natural level, which are potentially harmful to man and his biosphere are referred to as Air Pollutants. The examples of air pollutants are particulate matters of both organic and inorganic compounds, smoke, oxides of carbon, sulfur and nitrogen and radioactive tracers, etc. Smoke is mainly a mixture of gases and unburnt carbon particles resulting from incomplete combustion. Significant amounts of air pollutants are produced by combustion of fuels and the type of pollutant depends on the nature of fuel used. For example, if coal is used, fly ash, sulfur dioxide and oxides of nitrogen are the major pollutants. It may be noted that sulfur dioxide is relatively short-lived in the atmosphere and gets readily converted to sulfur trioxide which is even more reactive and combines rapidly with any available moisture to form sulfuric acid mist which is the primary culprit in the phenomenon of Acid Rain. Similar phenomenon occurs with the oxides of nitrogen forming nitric acid as well.

Air pollutants may be categorized according to their nature at the time of emission from the source and the chemical reaction in the atmosphere,

(i) Primary Pollutant : those directly emitted from a source or process, e.g., stack effluents, automobile exhaust.

(ii) Secondary Pollutant : those formed in the atmosphere by means of chemical interactions among two or more primary pollutants or other atmospheric constituents, e.g., photochemical smog, formation of acid mist.

Air pollutants are emitted in the atmosphere from various sources such as industrial stacks, power plants, automobile exhaust, burning of coal, fuel combustion, etc. These sources could be classified as point source (stacks), line source (highway vehicles) and area source (large industrial complexes).

#### 1.1.2 Effects of Air Pollution

The effects of air pollution to human health, to ecology, to our property and to our enjoyment are well known. Air pollution can cause bronchial asthma, chronic bronchitis and other respiratory and heart diseases. Carcinogenic agents cause cancer, dust particles cause respiratory diseases and heavy metals like lead may cause poisoning. Carbon monoxide combines with the hemoglobin in the blood causing stress on those suffering from cardiovascular and pulmonary diseases. Radioactive fallout may cause biological effects like genetic damage or mutation. The health effects on human beings, include eye irritation, nose and throat irritation and increase in the mortality and morbidity rate. Some specific pollutants and their effects on human health are listed below,

(i) Sulfur dioxide - an irritant, gas when inhaled affects the mucous membrane. Under certain conditions it oxidizes to sulfur trioxide which is much stronger irritant.

(ii) Carbon monoxide - has strong affinity for combining with the hemoglobin molecules of the blood forming carboxyhemoglobin (COHb) which reduces the overall capacity of the blood to carry oxygen to the cells.

(iii) Lead - emitted mainly from automobiles in urban atmosphere. Its effects include gastro-intestinal damage, liver and kidney damage, abnormalities in fertility and pregnancy and mental development of children.

(iv) Insecticides - can affect the central nervous system and may attack other vital organs. Undesirable effects of indoor spraying may affect domestic livestock.

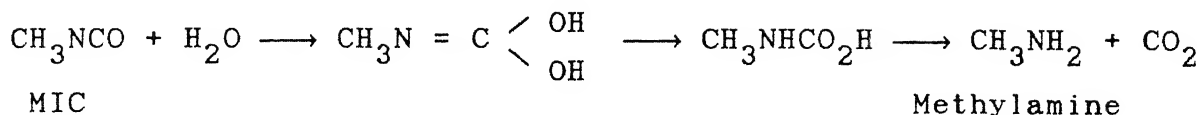
(v) Hydrocarbon vapors - formaldehyde is primarily irritating and contribute to eye and respiratory irritation caused by photochemical smog.

(vi) Radioactive isotopes - the major sources of radioactive air pollutants are nuclear reactors, testing of nuclear bombs in the atmosphere. The serious health effects are anemia, leukemia, and cancer, genetic defects and sterility as well as embryo defects and congenital malformations.

Human health and ecology are also affected by toxic gases released in the atmosphere due to accident and one of the most disastrous episode in the industrial history was that of Methyl isocyanate (MIC) gas leakage in a pesticide plant in Bhopal, 1984, India in which large number of people were reported to have suffered in different forms. Methyl isocyanate decomposes easily



with moisture forming methylamine, and is highly toxic and unstable. (Fieser and Fieser, 1961)



MIC affects all living beings including vegetation. In a report (Arora colony, 1984), the following types of effects were noticed when some people were exposed for 1-5 min.,

0.4 ppm	no effects
2.0 ppm	lachrymation, irritation in nose and throat
4.0 ppm	symptoms of irritation more marked
21.0 ppm	unbearable irritation of nose, eyes and throat

Prolonged exposure to MIC destroys proteins and lipids in the lungs which leads to changes in the permeability of the lung membrane, getting filled with water causing death. The maximum permissible limit of exposure for industrial workers is only 0.2 ppm for MIC, (Bretheric, 1981)...

Nuclear radiations from various sources constantly pose an environmental risk. A deadly mishap occurred due to nuclear device failure in Chernobyl, 1986, Russia, emitting huge amounts of radioactive material. This incident devastated a vast area around Chernobyl and gave rise to a nuclear cloud which remained cast over a large part of Europe for several days. In the case of a nuclear accident, dangerous radiations are emitted along with other harmful materials remaining in the atmosphere for a long time posing a threat to mankind. For example, an isotope of Strontium (Strontium-90) causes blood cancer and decays very slowly, Cesium-137 binds itself to soil and causes genetic changes and Iodine-131 has a tendency to cause thyroid cancer.

Air pollution has also an adverse effect on plants and vegetation interfering with the plant growth and photosynthesis. Smog, dust, etc., reduce the amount of light reaching the plants and clogging the stomata reducing the carbon dioxide intake. The leaves of the plants are severely affected by the pollutants in the form of necrosis, chlorosis, etc. The acid rain which is a major pollutant affects forests, vegetation, crops, monuments and causes acidification of water resources such as lakes, etc. destroying fish species and other marine ecosystems.

Air pollution is also associated with the damage of property as well as other economic losses. For example, due to pollutants, metal corrodes, rubber cracks and loses its elasticity, leather becomes brittle, glass is etched, dyed materials may fade, etc. The damage to materials are done mainly through abrasion, deposition on surfaces and by direct or indirect chemical attack. The Taj Mahal, a miracle in marble, is also facing serious threat due to commissioning of Mathura Oil Refinery about 40 kms. from the monument. Sulfur dioxide mixes with atmospheric moisture and gets converted to sulfuric acid which reacts with the marble (calcium carbonate) resulting in corrosion and decoloration of the monument.

The visibility may also be reduced due to formation of smog causing accidents, delay of flights, trains, etc. leading to economic losses.

## 1.2 DISPERSION OF AIR POLLUTANTS

The dispersion of air pollutants in the atmosphere is governed by the processes of molecular diffusion and convection and is mainly affected by various meteorological conditions such

as wind, temperature inversion, foggy atmosphere, topography of the terrain, etc. and types and number of sources. This process is also affected by several removal mechanisms such as chemical transformation, dry deposition, greenbelt plantation and precipitation scavenging, etc. In the study of pollutant dispersion, we are generally interested to find the concentration of the pollutant, after being emitted from its source, at a specified location and time. The concentration depends upon number of sources, their locations, emission rates and other meteorological and atmospheric conditions. Pasquill(1962), Ledbetter(1972), Dobbins(1979), Wark and Warner(1981), Seinfeld(1986), Shukla *et al.*(1987).

The hot plume from the stacks goes up to a certain height, called plume rise, into the atmosphere, due to buoyancy and momentum and then spreads in both horizontal and vertical directions by the dispersion process. This plume rise depends upon many factors like exit velocity, temperature of the plume, wind velocity and diameter of the stack, etc. The height of the stack is also an important factor in determining the level of pollution at a given location. The total sum of the actual stack height and the plume rise beyond the stack exit is termed as effective stack height.

#### 1.2.1 Diffusion Equation

Diffusion is the process by which matter is transported from one location in the atmosphere to another as a result of random molecular motions. The mathematical theory of diffusion in an isotropic media is based on Fick's law of diffusion which states that the rate of transfer of diffusing material through unit area

of cross section is proportional to the concentration gradient measured normal to the section, (Crank, 1975)

$$F = - D \frac{\partial C}{\partial x} \quad (1.1)$$

where  $F$  is the rate of transfer of diffusing material per unit area of cross section,  $C$  is the concentration of diffusing material and  $x$  is the space coordinate. Here  $D$ , the constant of proportionality, called the diffusion coefficient, depends upon many factors including the concentration. The diffusion equation in isotropic media may be written as, (in vectorial notation)

$$\frac{\partial C}{\partial t} = \text{div}(D \text{ grad} C) \quad (1.2)$$

where  $D$  may be function of  $x, y, z$ , the space coordinates, and  $C$ .

### 1.2.2 Convective Diffusion Equation

Assuming continuity in the atmosphere and noting the species balance, the convective diffusion equation or atmospheric transport equation can be derived as,

$$\begin{aligned} \frac{\partial C_i}{\partial t} + u \frac{\partial C_i}{\partial x} + v \frac{\partial C_i}{\partial y} + w \frac{\partial C_i}{\partial z} \\ = \frac{\partial}{\partial x} \left( K_x \frac{\partial C_i}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial C_i}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial C_i}{\partial z} \right) + R_i + S_i \\ i = 1, 2, 3 \dots \end{aligned} \quad (1.3)$$

where  $x, y, z$  are cartesian co-ordinates,  $t$  is the time,  $u, v, w$  are the components of the wind velocity in  $x, y$  and  $z$  directions respectively and  $K_x, K_y$  and  $K_z$  are turbulent diffusion coefficients. The terms  $R_i$  and  $S_i$  represent source (sink) and reaction (removal) terms, Dobbins(1979), Seinfeld(1986). The diffusion coefficients are, in general, functions of space variables and concentration, however, they may be taken as

constants for simplification. The source term can also be included in the boundary conditions rather than in the equation itself.

The above equation is widely used to study the dispersion of air pollutants with number of approximations and simplifications.

### 1.3 REMOVAL MECHANISMS

Various removal mechanisms are known to occur in the atmosphere which are effective in removing pollutants. Since the dispersal process is significantly affected by the removal mechanisms, it is absolutely essential to study the effects of removal mechanisms on the dispersion of air pollutants in the atmosphere. Some of the important removal processes are described below,

(i) Chemical transformation (reaction) - Many chemical reactions are known to occur in the atmosphere. Some of these may be very complex as that in the formation of photochemical smog. Others may be less complex as transformation of sulfur dioxide to acid rain. These chemical reactions are generally considered to be of first order and reduce the concentration of primary pollutants in the atmosphere. This mechanism can be used in removing the toxic species present in the atmosphere by introducing suitable liquid or gases which could react chemically with toxicants and neutralize their effects.

(ii) Dry deposition - The term dry deposition means direct collection of gaseous and particulate matter on earth's surface, soil or vegetative canopies. The deposition of pollutant species plays an important role in limiting the atmospheric concentration of the species. The vertical downward flux of a species is

represented in terms of an empirical parameter, called the deposition velocity  $v_d$ , multiplied by the concentration of the material at some height  $z_1$  i.e.,

$$\text{Flux} = v_d C(x, y, z_1, t) \quad (1.4)$$

where  $C$  is the concentration of the pollutant in the atmosphere. Modifying equation (1.1) for turbulent diffusion coefficient and using equation (1.4) one can write,

$$K_z \frac{\partial C}{\partial z} = v_d C(x, y, z, t) \quad \text{at } z = z_1 \quad (1.5)$$

This formalism applies to the diffusion of gases and fine particles when the gravitational settling velocity is negligible. The deposition velocity is certainly not a constant parameter and is subject to variability depending on the particular species or material that is being removed, on the meteorological parameters characterizing the state of surface layer, and on the nature of surface itself. Here  $v_d$  is a parameter that is proportional to the degree of absorptivity of the surface. At low emission heights, the removal of the pollutant by dry deposition must be taken into account in modelling process because under stable atmospheric conditions, the plume is restricted to a narrow boundary layer and the interaction of surface with plume can cause considerable mass removal.

The interaction between the diffusing material and the surface is mainly due to total absorption (i.e., if earth is a perfect absorber, the concentration of material at  $z = 0$  is zero) total reflection, and partial absorption where some particles are reflected and some are absorbed. The case of partial absorption at  $z = 0$  is given by, (as in equation 1.5)

$$K_z \frac{\partial C}{\partial z} = v_d C \quad \text{at } z = 0 \quad (1.6)$$

and for total reflection  $v_d = 0$  and  $v_d = \infty$  for total absorption.

If the effect of gravitational settling of pollutants (particulate matter), which, however, can be neglected for gases and particles smaller than approximately  $10 \mu\text{m}$  radius compared to turbulent diffusion, (Horst, 1984), is also to be included, the equation (1.5) modifies to

$$K_z \frac{\partial C}{\partial z} + w_s C = v_d C \quad \text{at } z = 0 \quad (1.7)$$

where  $w_s$  is the settling velocity of pollutants.

If there is an impermeable layer at  $z = H$  which inhibits vertical mixing, called the inversion layer, the boundary condition at  $z = H$  can be deduced from equation (1.5) as,

$$K_z \frac{\partial C}{\partial z} = 0 \quad \text{at } z = H \quad (1.8)$$

that is, when the effect of inversion is to be included, the condition at  $z \rightarrow \infty$  is simply replaced by a condition of zero flux in the  $z$ -direction at the inversion height provided there is no leakage in the inversion base.

(iii) Removal by greenbelt - The pollutants in the atmosphere can also be removed by suitable greenbelt plantation as plants have the capability of absorbing the pollutants. It may be mentioned here that the deposition, absorption characteristics of the greenbelt depend not only upon the distribution, size, height, nature of the canopy, etc. but also on the type of the pollutant, species of trees, shrubs, herbs, etc. planted in the greenbelt. Thus, the choice of the plantation should be such that the species planted be relatively resistant to the exposure of particular pollutant. The greenbelt acts like a sink for airborne material

because of its large surface area, the foliage of vegetative canopy serving as an effective receptor. If a greenbelt is planted suitably between the source and the region (i.e., a habitat, a historical monument, etc.) to be protected, it is possible to minimize the effect of pollution, the height of the source, thickness and the mean height of the greenbelt, determining the optimal location of the greenbelt.

(iv) Wet removal or precipitation scavenging - Precipitation scavenging (the process in which atmospheric gases/particulate matters are absorbed/trapped in rain droplets falling on the ground) provides important removal mechanism of pollutants from the atmosphere. This mechanism is sometimes subdivided into rainout (i.e., the process within clouds where plume expands freely into the cloud layer and material is 'removed' by getting dissolved in water or if it consists of particles, by getting entrapped in water droplets causing lowering of pollutant concentration) and washout (i.e., the process taking place below the cloud base for removal of airborne material by rain). Precipitation scavenging, not only acts like an important sink for trace gases in the atmosphere but also influences the local, regional and global distribution of air pollutants in the atmosphere.

#### 1.4 PATCHINESS IN THE ATMOSPHERE

It is pointed out here that the dispersal and removal processes are also affected by the ecological conditions on the ground and meteorological conditions in the atmosphere. For example, presence of a forest in a region would have different deposition rate affecting the dispersal process in comparison to



plains having little or no vegetation. Similarly these processes will be affected if rain is taking place in a region or it is covered by fog. Thus in real situations, the atmosphere may have patchiness with different dispersal, deposition and removal parameters in different patches and the modelling process must take this aspect into account.

## 1.5 OUTLINE OF THE RELEVANT LITERATURE : MODELLING THE FATE OF AIR POLLUTANTS IN THE ATMOSPHERE

As pointed out earlier, the dispersion of air pollutants is affected by meteorological conditions in the atmosphere, nature of terrain downwind from the stack, physical and chemical properties of the pollutant, number and location of stacks, etc. Several analytical studies have been conducted with some of the above mentioned factors but none of them accounts for all.

### 1.5.1 Simple models

The most comprehensive approach to transport theory is based on eddy diffusion model given by equation (1.3). The equation is quite complicated to solve analytically. It can be simplified to the following form,

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} + w \frac{\partial C}{\partial z} = K_x \frac{\partial^2 C}{\partial x^2} + K_y \frac{\partial^2 C}{\partial y^2} + K_z \frac{\partial^2 C}{\partial z^2} \quad (1.9)$$

by assuming constant diffusivity coefficients, no chemical reaction and other removal mechanisms in the atmosphere,

Using following assumptions,

- (i) The process is steady state, i.e.,  $\partial C / \partial t = 0$
- (ii) The wind speed  $u$  is constant at any point  $x, y, z$
- (iii) Major transport direction due to wind is along the  $x$  axis

(iv) The downwind diffusion is negligible in comparison to advection

equation (1.9) can be further simplified as,

$$u \frac{\partial C}{\partial x} = K_y \frac{\partial^2 C}{\partial y^2} + K_z \frac{\partial^2 C}{\partial z^2}, \quad K_y \neq K_z \quad (1.10)$$

The approximate solution to equation (1.10) under the following boundary conditions has been given by Lowry and Boubel(1967),

(i)  $C \rightarrow \infty$  as  $x \rightarrow 0$  i.e., concentration is large at the point source

(ii)  $C \rightarrow 0$  as  $x, y, z \rightarrow \infty$  i.e., concentration approaches zero at large distances from the source

(iii)  $K_z \frac{\partial C}{\partial z} \rightarrow 0$  as  $z \rightarrow 0$  i.e., no deposition on the surface  $z = 0$

(iv)  $\int_0^\infty \int_{-\infty}^\infty uC(x, y, z) dy dz = Q, x > 0$  i.e., rate of transport of pollutant downwind is constant and equal to the emission rate  $Q$  of the pollutant at the source, as follows:

$$C(x, y, z) = \frac{Q}{4\pi x (K_y K_z)^{1/2}} \exp \left[ -\frac{u}{4x} \left( \frac{y^2}{K_y} + \frac{z^2}{K_z} \right) \right] \quad (1.11)$$

$$r = (x^2 + y^2 + z^2)^{1/2}$$

The center line concentration at the ground level is given by,

$$C(x, 0, 0) = \frac{Q}{4\pi x (K_y K_z)^{1/2}} \quad (1.12)$$

which is inversely proportional to  $x$  and independent of wind speed  $u$ , the two departures when compared with the experimental evidence which shows that  $C$  is inversely proportional to  $(ux^{1.76})$ , (Wark and Warner, 1981). Equation (1.11) shows that away from the center line the concentration decays exponentially in both  $y$  and  $z$

directions. This mathematically means that C in the cross wind and vertical directions may be "normally" distributed. Also the decrease in the value of C in the x-direction is largely dependent on  $K_y$  and  $K_z$ , showing strong dependence on diffusion coefficients.

The other most widely accepted model which depends on the diffusion coefficients and exhibit the "normal" distribution as in equation (1.11) is the Gaussian plume model. The Gaussian plume model solution for a point source at the ground level in absence of any removal mechanisms is given by,

$$C(x,y,z) = \frac{Q}{\pi u \sigma_y \sigma_z} \exp \left[ -\frac{1}{2} \left( \frac{y^2}{\sigma_y^2} + \frac{z^2}{\sigma_z^2} \right) \right] \quad (1.13)$$

where Q is the source strength i.e., mass emitted per unit time and  $\sigma_y$ ,  $\sigma_z$  are the standard deviations of the concentration distributions related to mass diffusivities  $K_y$  and  $K_z$  as,

$$\sigma_y^2 = \frac{2K_y x}{u}, \quad \sigma_z^2 = \frac{2K_z x}{u}$$

The equation (1.13) is further modified to, if emission of a gaseous pollutant takes place from an elevated point source at an effective height  $h_s$ , without reflection at the ground

$$C(x,y,z) = \frac{Q}{2\pi u \sigma_y \sigma_z} \exp \left[ -\frac{1}{2} \left( \frac{y^2}{\sigma_y^2} + \frac{(z-h_s)^2}{\sigma_z^2} \right) \right] \quad (1.14)$$

However, for a reflection at the ground, it takes the following form,

$$C(x,y,z) = \frac{Q}{2\pi u \sigma_y \sigma_z} \exp \left( \frac{-y^2}{2\sigma_y^2} \right) \left[ \exp \left( \frac{-(z-h_s)^2}{2\sigma_z^2} \right) + \exp \left( \frac{-(z+h_s)^2}{2\sigma_z^2} \right) \right] \quad (1.15)$$

The above Gaussian plume equations, for non-reacting and

non-depositing pollutants from a continuous point source, in spite of their limited validity, have been extensively used for air pollution studies.

### 1.5.2 General models

Various investigations have been made to study the dispersion of air pollutants in the atmosphere under varying meteorological conditions such as wind, temperature inversion using both eddy diffusion models and Gaussian models. Smith(1957), Turner(1970), Peters and Klinzing(1971), Munn and Bolin(1971), Heines and Peters(1973a), Lamb and Seinfeld(1973), Nunge(1974a,b), Hameed(1974a,b), Yeh and Huang(1975), Ragland and Dennis(1975), Sander and Seinfeld(1976), Mehta and Balasubramanyam(1977,1978), Demuth(1978), Kao and Yeh(1979), Lupini and Tirabassi(1979,1983), Draxler(1980), Nieuwstadt(1980), Nieuwstadt and De Haan(1981), Wilson(1981), Llewelyn(1982), Karamchandani and Peters(1983), Robson(1983), Blondin(1984), Peterson(1985), Lorimer(1986), Lorimer and Ross(1986), Okamoto and Shiozawa(1987), Overcamp(1988), Lehmann(1989), Mihail *et al.*(1989), Kashibhatla and Peters(1990), Singh *et al.*(1990a,b), Eppel *et al.*(1991), Runca(1992), Pandey *et al.*(1992). In particular, Heines and Peters (1973a) presented an analytical model for continuously emitting infinite line and point sources with temperature inversion and constant wind velocity.

In general, the wind velocity and diffusivities are functions of space variables and time. When horizontal homogeneity is assumed, the wind velocity and diffusion coefficients may be taken as functions of height only. For general functional forms of these variables, no exact solutions of three dimensional diffusion

equation with chemical kinetics and other removal mechanisms are known. In a few cases when wind velocity and diffusivities are approximated, some solutions are available for two dimensional steady state equations. Smith(1957), Lebedeff and Hameed(1975) and Mehta and Balasubramanyam(1978) have studied the problem of steady state two dimensional advective diffusive transport of a non-reactive pollutant emitted from ground based area sources with variable wind and turbulent diffusivity approximated by power law profiles with no flux condition at the boundary of the contaminated layer. Lupini and Tirabassi(1979) have proposed a 'modified' Gaussian model for two dimensional steady state advective diffusion equation for a non-reactive pollutant emitted from an elevated point source and also studied the effect of plume trapping beneath an inversion by this 'modified' model. Nieuwstadt(1980) gave an analytical solution of the time dependent one-dimensional diffusion equation with more realistic diffusivity profiles than the power law profiles under stationary conditions for a non-reactive pollutant from an instantaneous area source assuming horizontal homogeneity in the atmosphere. Nieuwstadt and De Haan(1981) extended the above solution to non-stationary conditions in a developing boundary layer and applied the study to the special case of inversion-rise fumigation.

It may be noted here that the Gaussian puff models are useful to simulate the instantaneous releases whereas Gaussian plume models are used for continuous releases whose duration is significantly longer than the travel time to a receptor. Wilson(1981) has given extended version of the Gaussian plume model to account for ensemble-averaged along-wind diffusion of

time dependent source release rates and presented explicit solutions for a suddenly started release with exponential decay rate. Using moments method, Lupini and Tirabassi(1983) obtained approximate solutions of the advective diffusion equation for horizontally homogeneous atmospheric boundary layer for a passive pollutant emitted from an elevated instantaneous point source. Overcamp (1988) developed models to simulate transient releases with exponential decay, of a pollutant that undergoes first order decay. The models developed are based on one-dimensional diffusion in the downwind direction coupled with the conventional Gaussian model in the vertical and cross wind direction.

### 1.5.3 Effects of chemical reaction

As we have stated earlier in section 1.3 that many removal processes are known to exist in the atmosphere, the atmospheric dispersion models should, therefore, be modified to account for these removal mechanisms for more realistic dispersion phenomena. A few mathematical models are available that takes into account the effect of chemical transformation on dispersion of air pollutants e.g., Heines and Peters(1973b), Nunge and Vaidyanathan(1977), Peters and Richards(1977), Kewely(1978), Naresh and Nath(1990). Heines and Peters(1973b) have analytically studied the effect of a first order chemical reaction on steady state dispersion of air pollutants from a point or infinite line source under atmospheric inversion. Nunge and Vaidyanathan(1977) have also obtained analytical solution to the time dependent advective diffusion equation for dispersion of a reactive pollutant. Naresh and Nath(1990) have studied the effect of variability of chemical reaction on a two dimensional steady state

dispersion of air pollutant from ground based area sources with variable wind and diffusivity profiles and concluded that the concentration of the pollutant decreases as the rate of chemical reaction increases.

#### 1.5.4 Combined effects of chemical reaction, deposition and gravitational settling

The studies related to deposition of pollutants on the ground has also been taken up. Since it is expressed as a flux, it can be readily incorporated into a solution of advective diffusion equation as one of the required boundary condition. But in the case of Gaussian plume model, since it does not explicitly treat the vertical transport process, it is difficult to modify it for deposition that is realistic. Removal of pollutant by deposition in the Gaussian model was discussed by Chamberlain(1953) as noted in Van der Hoven(1968) referred to as the source-depletion model. Chamberlain(1953) assumed that the shape of the plume is not affected by the deposition but only its total content. The limitations of this method has been discussed by many authors e.g., Horst(1977), Prahm and Berkowicz(1978), Nordlund *et al.*(1979). The source-depletion model does not treat the vertical diffusive transport in accordance with the gradient transfer theory and neglects the effects of variation of diffusivity and wind with height. Assuming linear plume diffusion with downwind distance, Jensen(1980) presented relatively simple model including combined effect of diffusion and deposition. His, so called source-depletion model, however, becomes inferior to Horst's(1977) surface-depletion model especially under conditions where the atmospheric diffusion is slow and the deposition is fast. With

these limitations he gave explicit formulae for downwind deposition amounts and ground concentrations. Corbett(1981) discussed the source-depletion method, which is used to account for dry deposition in Gaussian plume models of the atmospheric dispersion of pollutants, on the basis of a diffusivity model and used these results to derive simple criteria for the validity of the method, which can be applied within the framework of the Gaussian model without explicit recourse to diffusivity theory. Bartzis(1983) extended the Gaussian model by incorporating the deposition effects for dispersion of radioactive material released from an elevated point source. His model, based on ideal diffusion problem, is rather more realistic than the widely used source-depletion model.

Numerous studies have been conducted to properly understand the phenomenon of deposition both mathematically and experimentally by taking into account the effects of deposition and also chemical reaction. Scriven and Fisher(1975a,b), Rasmussen *et al.*(1975), Höglström(1975), McMahon *et al.*(1976), Overcamp(1976), Slinn(1976), Ermak(1977), Garland(1977,1978), Horst(1977,1984), Berkowicz and Prahm(1978), Platt(1978), Astarita *et al.*(1979), Sehmel(1980), Alam and Seinfeld(1981), Davidson *et al.*(1981,1985), Carmichael and Peters(1984a,b), Renner *et al.*(1985), Bennet(1988), Shukla and Chauhan(1988), Chauhan and Shukla(1989), Koch(1989), Lehmann(1989), Noll and Fang(1989), Lovett and Kinsman(1990), Pandis and Seinfeld(1990), Underwood(1991a,b), Rao *et al.*(1992). The effect of gravitational settling of pollutants has also been studied e.g., Calder(1961), Smith(1962), Cleary *et al.*(1974), Ermak(1977), Peterson and



Seinfeld(1977), Fisher and Macqueen(1981), Rao(1982,1984), Lee(1985), Rao and Godowitch(1990). The dispersion of air pollutants when ground absorption and gravitational settling can not be ignored has been discussed by Calder(1961). In his formulation both the gravitational settling flux and the ground deposition flux are taken to be proportional to the local air concentration. Using this type of formulation, solutions to the atmospheric transport equation have been obtained for a number of cases. Rounds(1955), Smith(1962), Heines and Peters(1974). Using constant diffusivity and wind, Monin(1959) obtained an analytical solution of the diffusion equation including dry deposition. Scriven and Fisher(1975) gave an analytical solution for the cross-wind integrated concentration from an elevated continuous point source taking into account the dry deposition of the gaseous pollutant at the surface and its washout in rain. Ermak(1977) has solved the steady state three dimensional transport equation for an elevated continuous point source and obtained analytical solutions incorporating dry deposition and gravitational settling of the pollutants. Fisher and Macqueen(1981) have obtained steady state distribution for the integrated cross wind concentration of dust particulates emitted from an elevated point source including deposition and gravitational settling under inversion layer. Koch(1989) gave an analytical solution of the steady state two dimensional atmospheric diffusion equation with dry deposition using power law profiles for wind velocity and vertical diffusion coefficient in an unbounded atmosphere while Lehmann(1989) presented a solution of time dependent one-dimensional diffusion equation for an inert pollutant from an elevated point source

incorporating dry deposition at the ground and leakage at the top of the inversion layer for simple diffusion coefficient profiles and illustrated them numerically. Rao and Godowitch(1990) have briefly described a methodology to include the combined effect of deposition, gravitational settling and first order chemical transformation in urban air pollution models. The concentration expressions given by him can be thought of as analytical extensions of the familiar Gaussian plume dispersion models with these removal mechanisms.

It is well known that a primary pollutant is often converted to a secondary pollutant in the atmosphere, (e.g.,  $\text{SO}_2$  is converted to  $\text{SO}_4^{--}$ ) which is even more deleterious. In this direction, Alam and Seinfeld(1981) have studied the dispersion of sulfur dioxide and sulfate from a point source by taking into account the dry and wet removal of both the species and obtained analytical solutions of the steady state, coupled, three dimensional atmospheric diffusion equation incorporating first order chemical conversion and removal under inversion conditions. Similar problem including combined effect of settling, deposition, first order removal and conversion of gaseous to particulate pollutant has been studied by Peterson and Seinfeld (1977). Lee(1985) also gave analytical solutions for both primary and secondary pollutants including above mentioned factors in an unbounded atmosphere i.e., without inversion.

It is pointed out here that these problems, where deposition, sedimentation, etc. are taken into account, have been studied under steady state conditions only but the sources of the pollutant could be time dependent e.g., explosion of a nuclear

device, leakage of toxic gases from storage tanks, etc. In such cases unsteady state atmospheric diffusion equation with above removal mechanisms should be considered, e.g., Cleary *et al.*(1974), Llewelyn(1983), Shukla and Chauhan(1988). In particular, Shukla and Chauhan(1988) have solved unsteady state, coupled, three dimensional convective diffusion equation for a reactive pollutant emitted from a time dependent point source forming secondary species in the atmosphere by taking into account the dry and wet deposition of pollutant for different forms of flux at the point source and applied the analysis to study the dispersion of MIC leakage at Bhopal, India.

A thorough review of long range transport models and processes with regard to dry deposition and other removal mechanisms have also been described by some workers which are of special interest may be noted, e.g., Scriven and Fisher(1975a,b), Fisher(1975,1981,1983), Eliassen (1980), Fay and Rosenzweig(1980), Slinn(1982b), Fisher and Smith(1987), Janssen and Asman(1988).

In view of the above literature survey, it may be pointed out that the unsteady state dispersion of pollutant in the atmosphere has not been studied in a patchy atmosphere. Therefore, in chapters II and III of the thesis, we have studied the unsteady state dispersion of a reactive air pollutant from a time dependent point source forming secondary species for different forms of flux at the source by taking into account the first order chemical conversion of primary pollutant to secondary pollutant, removal process, deposition at the ground, leakage at the inversion height, gravitational settling, etc. in a two patch environment under inversion conditions.

### 1.5.5 Effect of greenbelt

The concentration of pollutants in the atmosphere can be reduced considerably by plantation of greenbelt suitably at a required place to protect the region under consideration (a historical monument, a habitat). It is well established that certain plants have the capability of removing the pollutants by absorption, deposition, etc. and these characteristics of greenbelt depend upon many factors like distribution, size, height, nature of the canopy, etc. and also on the type of the pollutant, species of trees, shrubs, herbs, etc. planted in the greenbelt. In fact the choice of the plantation should be such that the species planted be relatively resistant to the exposure of particular pollutant. Several studies to study the effect of various pollutants on different plant species have been made in the last few decades or so, e.g., Thomas and Hendricks(1956), Todd and Garber(1958), Brandt and Heck(1968), Treshow(1968), Daines(1968), Davis(1972), Garsed *et al.*(1981), Takemoto and Noble(1982), Dochinger(1988), Evans(1988). It may be noted that there are plants which are relatively resistant to specific pollutants. In particular, survey of Indian plants in relation to atmospheric pollutants have been conducted by Ahmad *et al.*(1988). They have found forty eight species of pollutant tolerant trees, shrubs and herbs that thrive well in the polluted environments and have been recommended for landscaping urban and industrial areas for mitigating air pollution. Some of them are listed here, Neem(*Azadirachta indica*), Kadamb(*Anthocephalus cadamba*), Shisham (*Dalbergia sissoo*), Tendu(*Diospyros melanoxylon*), Sahjan(*Moringa oleifera*), Ashok(*Polyalthia longifolia*), Jamun(*Syzygium cuminii*),

Kaner(*Nerium odorum*), *Amaranthus graecizans*.

The transport of gases and particulate matters within plant and vegetative canopies has been studied by many researchers, MacBean(1968), Hill(1971), Bennet and Hill(1973,1975), Hartog and Shaw(1974), Raynor *et al.*(1974), Shaw *et al.*(1974), Aylor(1975), Chamberlain(1975a,b), Petit *et al.*(1976), O'Dell *et al.*(1977), Bache(1979a,b), Smith(1981), Hosker and Lindberg(1982), Slinn(1982a), Kapoor and Gupta(1984), Wiman and Agren(1985), Wiman and Lannefors(1985), Wiman *et al.*(1985), Baldocchi *et al.*(1987), Shukla and Chauhan(1987), Lindberg and Lovett(1992), Lovett and Lindberg(1992). In particular, Petit *et al.*(1976) presented some results concerning characteristics of air flow within and above a forest and calculated SO<sub>2</sub> fluxes at the top of the canopies. He aimed at determining the behavior of the forest towards SO<sub>2</sub> and to develop a diffusion model of SO<sub>2</sub> with associated absorption by the roughness. Bache(1979a,b) has also developed an analysis and suggested a modified form of turbulent diffusion equation to take into account the particulate transport behavior within plant canopies. A theoretical framework to predict particle deposition due to vegetation by considering variable wind velocity profile has been given by Slinn(1982a). A review of atmospheric deposition regarding plant assimilation of gases and particles has been presented by Hosker and Lindberg(1982) and Smith(1981). Wiman and Agren(1985) proposed a mathematical model for aerosol depletion and deposition on forests by considering a modified form of convective diffusion equation. His model considers the interaction between forest structure, open field, forest aerodynamics and aerosol characteristics.

From these studies it may be speculated that if a greenbelt (in the form of forest capable of absorbing the pollutant) is provided suitably between the source and the region to be protected, it is possible to minimize the effect of pollution on the region under consideration. In this direction Kapoor and Gupta(1984) have studied the attenuation of an inert pollutant by a greenbelt under steady state conditions.

It may be noted here that no information is available on concentration reduction due to greenbelt plantation when the pollutant is emitted from time dependent sources as well as the effect of inter-exchange process near the canopy surface. In view of this in chapter IV, the effect of greenbelt on the concentration reduction of a reactive air pollutant emitted from a time dependent point source with different forms of flux is studied. Also the optimum location of greenbelt between the source and the receptor (i.e., the area to be protected) is found for the maximum concentration reduction at the receptor.

#### 1.5.6 Effect of precipitation scavenging

In the last few decades increased number of investigations have also been carried out to understand the scavenging of pollutants/contaminants by precipitation. Engelmann (1968), Postma (1970), Engelmann and Slinn(1970), Hales (1972,1978,1982,1989), Hales *et al.*(1973), Dana *et al.*(1973,1975), Slinn(1974,1977,1978), Davies(1976), Peters(1976), Barrie(1978), Garland(1978), Maul(1978), Radke *et al.*(1980), Rodhe(1980), Fisher(1982), Levine and Schwartz(1982), Shukla *et al.*(1982), Chang(1984), Kumar(1985,1986,1989), Shukla and Chauhan(1987), Luecken *et al.*(1989), Tsai *et al.*(1990). In particular, Postma(1970) and

Hales(1972) presented some fundamentals for the general analysis of precipitation scavenging emphasizing the importance of reversible phenomenon. Since the process of trace gas scavenging is reversible in nature and the phenomenon of absorption and desorption may cause a redistribution of pollutants in the atmosphere as pointed by Hales(1972), Slinn(1974) has analytically considered the redistribution of gas plume caused by reversible washout and presented solutions in some simple cases. A simplified linearised model for predicting reversible gas washout of pollutant from industrial plumes has been presented by Hales *et al.*(1973) considering rain to be composed of spherical, non-interacting drops of static size distribution. Peters(1976) presented a theoretical analysis of the contribution to rain water sulfate concentration by precipitation scavenging of gaseous  $\text{SO}_2$  and sulfate containing aerosols. The reversible rain washout of soluble gases such as sulfur dioxide, Ammonia and carbon dioxide has been studied by a number of authors, e.g., Dana *et al.*(1975), Hill and Adamowicz(1977), Adeuyi and Carmichael(1982). Shukla *et al.*(1982) have calculated vertical concentration distribution of a gaseous pollutant emitted at ground level into a stagnant fog layer containing uniform distribution of fog droplets by assuming reversible absorption of a pollutant species. Fisher(1982) has studied the transport and removal of sulfur dioxide in rain using a simple model which combines the microphysics of absorption and chemical transformation of sulfur dioxide in clouds with the dynamics of the air motion and obtained approximate one dimensional solution of the governing equations. A detailed theory of  $\text{HNO}_3$  vapor removal (particularly, below-cloud removal by rain)

has been carried out by Levine and Schwartz(1982). Chang(1984) has derived wet removal coefficients for  $\text{HNO}_3$  vapor in rain and snow systems and parameterized them in terms of precipitation rate, under a number of approximations. Since the concentration of the pollutant in gaseous phase directly influence the concentration of the pollutant in droplet phase it is, therefore, necessary to consider simultaneously the coupled process of gas phase depletion and aqueous phase accumulation of the pollutant. Kumar(1985) has given an Eulerian model to describe the simultaneous process of trace gas removal from the atmosphere and absorption of these gases in rain drops by considering the precipitation scavenging of these gases present below the cloud base but his model does not take into account the wind velocity and the presence of a continuous source. He (1986) has extended the above model to take into account the process of absorption of multiple species and chemical reactions within the droplets.

In the above studies the transient emission of pollutant from the source as well as the non-linear interaction between the primary and secondary pollutants with the time dependent distribution of rain droplets have not been taken into account. In view of this in chapters V-VI, we have studied the effect of precipitation scavenging on concentration distribution of a reactive air pollutant from a time dependent point source for different forms of flux at the source. In these studies we have considered two phases in the atmosphere i.e., the pollutant phase and the phase of absorbed pollutant in the droplets whereas in chapter VII we have proposed a nonlinear ecological type model to study the effect of precipitation scavenging on the concentration



distribution of primary and secondary pollutant using stability theory.

## 1.6 SUMMARY OF THE WORK DONE IN THE THESIS

The thesis consists of seven chapters and deals with the unsteady state dispersion of a reactive air pollutant emitted from a time dependent point source with different forms of flux at the source. The main concern has been to discuss the effects of removal mechanisms such as chemical transformation, dry deposition, removal by greenbelt and precipitation scavenging on the dispersion process. In these studies, the unsteady state convective diffusion equations both for primary and secondary pollutants have been solved with appropriate initial and boundary conditions. The effect of patchiness in the atmosphere on the dispersion process has also been studied. It is assumed that the wind is sufficiently large to neglect the downwind diffusion. A nonlinear model is also proposed for removal mechanism of both primary and secondary pollutants due to precipitation scavenging using ecological type ideas in the last chapter of the thesis.

In chapter I a general introduction and basic concepts of air pollution with relevant literature is presented to provide a necessary feedback required for the forthcoming chapters.

In chapter II the unsteady state dispersion of a reactive air pollutant emitted from a time dependent point source forming secondary pollutant is studied by taking into account the first order conversion of primary pollutant to secondary pollutant in a two patch environment, assuming the existence of sinks, uniformly distributed throughout the second patch, causing the removal of both primary and secondary pollutants. These sinks in the

here may represent rain droplets, fog droplets or even  
 ally introduced species (liquid or gas) which are effective  
 removal of pollutants by chemical reaction, etc. The latter  
 s may be useful in removing the toxic species in the  
 here by accidental releases from an instantaneous source.  
 oblem is studied by solving unsteady state, coupled, three  
 onal convective diffusion equations in both the patches for  
 primary and secondary pollutants with removal terms  
 rating the deposition at the ground and the leakage at the  
 on layer with suitable matching at the interface of the two  
 . The time dependent flux at the source is considered to be  
 forms, (i) Instantaneous (ii) Constant, and (iii) Step  
 a type.

e effects of removal mechanisms on the concentration  
 tion of both the species are then discussed in all the  
 uses of time dependent flux at the source. It is observed  
 e concentration of pollutants decreases as downwind  
 increases in all the three cases. Also the concentration  
 ry pollutant decreases but that of secondary pollutant  
 s at a particular time and location as the rate of  
 on of primary pollutant to secondary pollutant increases.  
 ound that the central line concentration of both the  
 ts decreases as time increases for instantaneous flux  
 it increases as time increases, and reaches their  
 e steady state values for constant flux. When flux is  
 tion type, the concentration characteristics of both the  
 s are similar to the combined effect of the above two  
 . is noted that the concentration of both the pollutants

decreases considerably due to removal parameter associated with the sink phase.

From the analysis it is concluded that the presence of sink phase in the second patch in the form of rain droplets, fog droplets or even externally introduced species can be very effective in removing the pollutants from the atmosphere. The analysis thus suggests a mechanism by which toxic gases leaked out in the atmosphere due to accidental discharge, etc. can be neutralized by introducing suitable liquid or gas phase in the atmosphere by mechanical means. The analysis can also be utilized for studies related to risk analysis particularly in cases of accidental leakage of toxicants/pollutants such as MIC leakage in a pesticide plant, Bhopal, India.

In chapter III we study the unsteady state dispersion of both primary and secondary pollutants, which are heavier than air, in a two patch environment to see the effect of gravitational settling, on the dispersion of these pollutants. The deposition of settling particles at the ground and the removal of these pollutants have been taken into account. As in chapter II, the relevant equations with settling terms have been solved and it is found that the concentration of the pollutants decreases when gravitational settling velocity increases for the points above the source height, however, for the points below the source height, result is just reversed. This is expected because after emission of pollutants from the source gravity comes into effect and heavier particles are likely to have higher settling velocity in comparison to not so heavier particles. The effect of removal is, however, to decrease the concentration of both the pollutants.

Chapter IV deals with the effect of greenbelt (plantation capable of absorbing the pollutant and inducing deposition) on dispersion of a reactive air pollutant from a time dependent point source under atmospheric inversion condition. The inversion layer is divided into four regions where source is located in the first region and the greenbelt lies some distance away from the source in downwind direction in the second region. The region above the greenbelt is the third region whereas the region next to greenbelt in downwind direction is the fourth region i.e., the region, where the receptor (a historical monument, a habitat, etc.) is located. The vertical and horizontal diffusion processes in the greenbelt region are assumed to be negligible due to denseness of the plant canopies and shrubs grown on the ground below canopies of the plants. It is assumed further that the entire greenbelt is acting as a sink for the pollutant under consideration. The wind velocity, diffusion coefficients and deposition rates are taken to be different in all the four regions. The relevant equations with above assumptions have been solved within and outside the greenbelt using appropriate boundary and matching conditions with suitable deposition condition at the top of the greenbelt. The analysis has also been done for the case where inter-exchange process is taken into account, in a narrow zone of the third region adjacent to the top of the greenbelt, characterized by an exchange velocity. It is found that the concentration of the pollutant decreases considerably in presence of greenbelt. The optimization of the location of greenbelt is also studied to affect the maximum concentration reduction on the receptor in the above cases. It is seen that, when the source height is greater

han the greenbelt height, the greenbelt should be located close o the receptor and when the source height is less than or equal o the greenbelt height, it should be located near the source .e., if sources are ground based like storage tanks it is esirable to surround this area by the greenbelt to avoid the ollutant spreading in the case of an accidental blast. The effect f other removal parameters like deposition, depletion coefficient ue to greenbelt, inter-exchange velocity, etc. is to decrease the oncentration of the pollutant.

Chapter V deals with the study of the effect of precipitation cavenging on the dispersion of a reactive pollutant emitted from time dependent point source. It is assumed that the rain roplets are uniformly distributed in the atmosphere which absorb he pollutant and remove it by their fall on the ground with a onstant velocity. We consider that the concentration of the ollutant in the gaseous phase is governed by the unsteady state hree dimensional convective diffusion equation with removal terms hereas the concentration of the absorbed pollutant in droplet hase is assumed to be governed by a simplified equation which akes into account the falling of rain droplets but neglects the iffusion, the case applicable to the heavy monsoon rain. These quations are then solved using suitable initial and boundary onditions and the expressions are obtained for the concentration istribution of pollutant in gaseous phase and in rain droplet hase. The forms of time dependent flux at the point source are aken to be (i) Instantaneous, and (ii) Constant. It is shown that he concentration of the pollutant in the atmosphere reduces onsiderably, under appropriate conditions, due to precipitation

scavenging by rain, thus providing an important mechanism for removing pollutants/toxicants from the atmosphere.

In chapter VI a similar problem of removal of pollutant by precipitation scavenging is studied in a two patch environment. It is assumed that the rain is taking place, some distance away from the source in the second patch where the effect of precipitation scavenging is studied. It is shown that, as the pollutant front reaches in the second patch where rain is taking place, the concentration of pollutant reduces significantly due to washout process for both the cases of instantaneous and constant flux at the source.

Finally, from the above analysis and the results in chapter V, it may be concluded that precipitation scavenging is a very important mechanism for the removal of pollutant from the atmosphere at a given receptor point located in the second patch. However, the rate of reduction depends upon the location of the patch and prevailing meteorological conditions. It is also noted that the reduction in pollutant concentration is larger at this receptor when precipitation patch is closer to the source.

Since in real situations during precipitation, the number density of rain, fog or snow droplets changes as the intensity of precipitation increases and this change in number density affects the interaction process and should, therefore, be taken into account in the model. Thus, In chapter VII a nonlinear model is proposed for removal mechanism of both primary and secondary pollutants, due to precipitation scavenging, by taking into account the interaction of the droplet phase with the pollutant phase. In fact, we consider that there exist four separate

nonlinearly interacting phases, (i.e., the droplet phase, primary pollutant phase, secondary pollutant phase and the combined phase of both the pollutants absorbed in droplets). We assume that in these phases, the number density of droplets, the concentration of both primary and secondary pollutants and the concentration of both the pollutants absorbed in the droplets are governed by evolution equations (i.e., nonlinear ordinary differential equations) with source and removal terms. It is assumed that the rate of removal of pollutants is proportional to the concentration of pollutants as well as the number density of droplets in the atmosphere. Further, the concentration of pollutants absorbed depends nonlinearly on the number density of droplets as well as the concentration of both the pollutants. Our aim here is to analyze the proposed nonlinear model and to see the effect of removal mechanism on the equilibrium level of pollutants in the atmosphere. The analysis is done for both cases of with and without secondary pollutant. To understand the removal mechanism, Liapunov's stability is used. It is shown that when the pollutant is emitted by an instantaneous source (single introduction of the pollutant in the atmosphere), both the pollutants would be removed completely from the atmosphere by the precipitation process. When the pollutant is emitted at a constant rate, it is found that the pollutants may be removed from the atmosphere completely but it would depend upon the rate of emission and other removal processes.

## CHAPTER II

# UNSTEADY STATE DISPERSION OF A REACTIVE AIR POLLUTANT FROM A TIME DEPENDENT POINT SOURCE FORMING SECONDARY SPECIES IN A TWO PATCH ENVIRONMENT

## 2.0 INTRODUCTION

In the environment various mechanisms, such as chemical reaction, dry deposition on the ground and on vegetative canopies and precipitation scavenging by rain, fog or snow, are known to exist and are effective in the removal of pollutants from the atmosphere. In the last few decades several investigations have been conducted to study the dispersion of air pollutants in the atmosphere under various meteorological conditions with different kinds of removal mechanisms, Scriven and Fisher(1975a,b), McMahon *et al.*(1976), Alam and Seinfeld(1981), Shukla *et al.*(1982), Robson(1983), Llewelyn(1983), Seinfeld(1986), Shukla and Chauhan(1988), Chauhan and Shukla(1989), Lehmann(1989), Shukla *et al.*(1991b) including scavenging by rain droplets, Hales(1972), Hales *et al.*(1973), Slinn(1974), Kumar(1985).

It is known that primary pollutant is often converted to secondary pollutant in the atmosphere (e.g.,  $\text{SO}_2$  is converted to  $\text{SO}_4^{--}$ ) and both of these are required to be removed from the atmosphere. In this direction Alam and Seinfeld(1981) have studied

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the dispersion of sulfur dioxide and sulfate from a point source by taking into account the dry and wet deposition of both the species and obtained analytical solution of steady state, three dimensional atmospheric diffusion equation incorporating the first order conversion and removal. Shukla and Chauhan(1988) have also studied the similar problem under unsteady state conditions when the pollutant is emitted from a point source, with different forms of time dependent flux and applied the analysis to the study of dispersion of MIC leakage in a pesticide plant in Bhopal, 1984, India.

As pointed out in chapter I, in real situations, the ecological conditions on the ground and meteorological conditions in the atmosphere are different at different places leading to patchiness in the environment with different dispersal, deposition and removal parameters in each patch. This aspect has not been studied in the above investigations.

In this chapter we, therefore, study the unsteady state dispersion of air pollutant emitted from a time dependent point source forming secondary species by taking into account the effects of removal mechanism in a two patch environment, assuming the existence of sinks uniformly distributed throughout the second patch causing the removal of both the primary and secondary pollutants. In the atmosphere these sinks may represent rain droplets, fog droplets or even externally introduced species (liquid or gas) which are effective in the removal of pollutants by chemical reactions, etc. The latter process may be useful in removing the toxic species in the atmosphere by accidental

releases from instantaneous sources. This problem has been studied by solving coupled three dimensional unsteady state convective diffusion equations involving both primary and secondary pollutants with removal terms and incorporating the deposition at the ground and the leakage at the top of the inversion layer with suitable matching at the interface of the two patches. The forms of time dependent flux at the point source considered in the analysis are: (i) Instantaneous, (ii) Constant, and (iii) Step function type.

The effects of removal mechanism in the second patch on the concentration distribution of both primary and secondary species are discussed in all the above cases.

## 2.1 MATHEMATICAL MODEL

Consider the dispersion of a reactive air pollutant, undergoing first order chemical conversion and removal, from a time dependent point source of strength  $Q(t)$  located at height  $h_s$  from the ground  $z = 0$ , forming secondary species in a two patch environment under atmospheric inversion as shown in Figure 2.1. The source of secondary pollutant is, however, the transformation of primary pollutant. It may be noted that the time dependent source is located in the first patch where some kind of removal mechanism may exist, however, in the second patch it is assumed that there exist a phase of uniformly distributed sinks as described earlier which are mainly responsible for removing both the primary and secondary pollutants from the atmosphere. In the two patches wind velocity, deposition and other removal parameters are taken to be different. It is also assumed that the wind is

sufficiently large in both the patches so that downwind diffusion is negligible in comparison to advection.

Under these assumptions the partial differential equations governing the concentration of pollutants in both the patches, with appropriate initial and boundary conditions can be written as follows,

Patch I  $(0 \leq x < x_1, 0 \leq z \leq H)$

The differential equation governing the concentration  $C_1(x,y,z,t)$  of the primary pollutant in the first patch is written as,

$$\frac{\partial C_1}{\partial t} + u_1 \frac{\partial C_1}{\partial x} = K_{y1} \frac{\partial^2 C_1}{\partial y^2} + K_{z1} \frac{\partial^2 C_1}{\partial z^2} - (k_1 + k_{g1})C_1 \quad (2.1)$$

where  $x, y, z$  are cartesian co-ordinates,  $t$  is the time,  $x$ -axis is taken in the downwind direction and  $z$ -axis vertically upwards,  $u_1$  is the mean wind velocity,  $K_{y1}$  and  $K_{z1}$  are diffusivities in  $y$  and  $z$  directions respectively, taken as constants. The constant  $k_1$  is the conversion rate coefficient of primary pollutant to secondary pollutant and  $k_{g1}$  is its removal rate coefficient.

We prescribe the following initial and boundary conditions for equation (2.1),

The initial concentration distribution of the pollutant is assumed to be zero,

$$C_1(x,y,z,t) = 0 \quad \text{at } t = 0 \quad (2.2)$$

A point source of strength  $Q(t)$  is assumed to be located at  $(0,0,h_s)$ . Thus the condition at  $x = 0$  is,

$$C_1(x,y,z,t) = \frac{Q(t)}{u_1} \delta(y) \delta(z-h_s) \quad \text{at } x = 0 \quad (2.3)$$

At infinite lateral distance the concentration approaches zero,

$$C_1(x,y,z,t) = 0 \quad \text{as } y \rightarrow \pm \infty \quad (2.4)$$

The pollutant may also be removed by the deposition process at the ground  $z = 0$ ,

$$K_{z1} \frac{\partial C_1}{\partial z} = v_{d1} C_1 \quad \text{at } z = 0 \quad (2.5)$$

The pollutant may also 'escape' into the base of the inversion layer at  $z = H$ , which is taken into account as,

$$K_{z1} \frac{\partial C_1}{\partial z} = -w_1 C_1 \quad \text{at } z = H \quad (2.6)$$

where  $v_{d1}$  is the deposition velocity of the primary pollutant at  $z = 0$ , which in general depends on the particular species or material that is being removed and on the prevailing meteorological conditions and  $w_1$  is its leakage velocity at  $z = H$ , the height of the inversion layer, a layer of stable air which forms a barrier to vertical mixing and  $\delta(.)$  is the Dirac delta function.

Similarly the differential equation governing the concentration  $C_{p1}(x,y,z,t)$  of the secondary pollutant can be written as,

$$\frac{\partial C_{p1}}{\partial t} + u_1 \frac{\partial C_{p1}}{\partial x} = K_{y1} \frac{\partial^2 C_{p1}}{\partial y^2} + K_{z1} \frac{\partial^2 C_{p1}}{\partial z^2} + k_1 C_1 - k_{p1} C_{p1} \quad (2.7)$$

The initial and boundary conditions for equation (2.7) are, (assuming that there is no direct emission of secondary pollutant

from the source)

$$C_{p1}(x,y,z,t) = 0 \quad \text{at} \quad t = 0 \quad (2.8)$$

$$C_{p1}(x,y,z,t) = 0 \quad \text{at} \quad x = 0; y = 0, z = h_s \quad (2.9)$$

$$C_{p1}(x,y,z,t) = 0 \quad \text{as} \quad y \rightarrow \pm \infty \quad (2.10)$$

$$K_{z1} \frac{\partial C_{p1}}{\partial z} = v_{dp1} C_{p1} \quad \text{at} \quad z = 0 \quad (2.11)$$

$$K_{z1} \frac{\partial C_{p1}}{\partial z} = -w_{p1} C_{p1} \quad \text{at} \quad z = H \quad (2.12)$$

where  $k_{p1}$  is the removal rate coefficient of the secondary pollutant,  $v_{dp1}$  is its deposition velocity at  $z = 0$  and  $w_{p1}$  is the leakage velocity at  $z = H$ .

Patch II ( $x \geq x_1, 0 \leq z \leq H$ )

The differential equation governing the concentration  $C_2(x,y,z,t)$  of the primary pollutant in the second patch is written as,

$$\frac{\partial C_2}{\partial t} + u_2 \frac{\partial C_2}{\partial x} = K_{y2} \frac{\partial^2 C_2}{\partial y^2} + K_{z2} \frac{\partial^2 C_2}{\partial z^2} - (k_2 + k_{g2} + \delta_1) C_2 \quad (2.13)$$

where  $u_2$  is the mean wind velocity,  $K_{y2}$  and  $K_{z2}$  are diffusivities in  $y$  and  $z$  directions respectively,  $k_2$  is the conversion rate coefficient of primary pollutant to secondary pollutant,  $k_{g2}$  is its removal rate coefficient and  $\delta_1$  is the depletion rate coefficient due to uniformly distributed sinks, the magnitude of which may increase if number or size of sinks increases.

The initial and boundary conditions for equation (2.13) are,

$$C_2(x,y,z,t) = 0 \quad \text{at} \quad t = 0 \quad (2.14)$$

$$C_2(x,y,z,t) = C_1(x,y,z,t) \quad \text{at } x = x_1 \quad (2.15)$$

$$C_2(x,y,z,t) = 0 \quad \text{as } y \rightarrow \pm \infty \quad (2.16)$$

$$K_{z2} \frac{\partial C_2}{\partial z} = v_{d2} C_2 \quad \text{at } z = 0 \quad (2.17)$$

$$K_{z2} \frac{\partial C_2}{\partial z} = -w_2 C_2 \quad \text{at } z = H \quad (2.18)$$

where  $v_{d2}$  is the deposition velocity of the primary pollutant at  $z = 0$  in the second patch and  $w_2$  is its leakage velocity at  $z = H$ .

Similarly the differential equation governing the concentration  $C_{p2}(x,y,z,t)$  of the secondary pollutant can be written as,

$$\frac{\partial C_{p2}}{\partial t} + u_2 \frac{\partial C_{p2}}{\partial x} = K_{y2} \frac{\partial^2 C_{p2}}{\partial y^2} + K_{z2} \frac{\partial^2 C_{p2}}{\partial z^2} + k_2 C_2 - (k_{p2} + \delta_2) C_{p2} \quad (2.19)$$

The initial and boundary conditions for equation (2.19) are,

$$C_{p2}(x,y,z,t) = 0 \quad \text{at } t = 0 \quad (2.20)$$

$$C_{p2}(x,y,z,t) = C_{p1}(x,y,z,t) \quad \text{at } x = x_1 \quad (2.21)$$

$$C_{p2}(x,y,z,t) = 0 \quad \text{as } y \rightarrow \pm \infty \quad (2.22)$$

$$K_{z2} \frac{\partial C_{p2}}{\partial z} = v_{dp2} C_{p2} \quad \text{at } z = 0 \quad (2.23)$$

$$K_{z2} \frac{\partial C_{p2}}{\partial z} = -w_{p2} C_{p2} \quad \text{at } z = H \quad (2.24)$$

where  $k_{p2}$  is the removal rate coefficient of the secondary pollutant,  $\delta_2$  is the depletion rate coefficient of secondary pollutant due to sinks,  $v_{dp2}$  is the deposition velocity of it at

$z = 0$  and  $w_{p2}$  is its leakage velocity at  $z = H$ . The following forms of flux  $Q(t)$  at the source are considered in the subsequent analysis,

(i) Flux is Instantaneous

$$Q(t) = Q_0 \delta(t)$$

(ii) Flux is Constant

(2.25)

$$Q(t) = Q_c (\text{constant})$$

(iii) Flux is Step function type

$$Q(t) = Q_c \quad 0 \leq t \leq t_0 \\ = 0 \quad t > t_0$$

where  $Q_0$  is constant.

It is convenient to cast the problem in dimensionless form. For that we use the following dimensionless quantities,

$$\bar{t} = \frac{K_{z0} t}{H^2}, \quad \bar{x} = \frac{K_{z0} x}{u_0 H^2}, \quad \bar{y} = \frac{y}{H}, \quad \bar{z} = \frac{z}{H}, \quad \bar{h}_s = \frac{h_s}{H}, \quad \bar{u}_i = \frac{u_i}{u_0}$$

$$\bar{C}_i = \frac{u_0 H^2}{Q_c} C_i, \quad \bar{C}_{pi} = \frac{u_0 H^2}{Q_c} C_{pi}, \quad \bar{Q}(t) = \frac{Q(t)}{Q_c}, \quad \bar{Q}_0 = \frac{Q_0}{Q_c} \frac{K_{z0}}{H^2},$$

$$\bar{\delta}_i = \frac{H^2 \delta_i}{K_{z0}}, \quad i = 1, 2$$

where  $K_{z0}$  and  $u_0$  are reference diffusion coefficient and wind velocity respectively.

The equations (2.1)-(2.25) can be written in dimensionless form (dropping bars for convenience) as :

Patch I ( $0 \leq x < x_1, \quad 0 \leq z \leq 1$ )

$$\frac{\partial C_1}{\partial t} + u_1 \frac{\partial C_1}{\partial x} = \beta_1 \frac{\partial^2 C_1}{\partial y^2} + \gamma_1 \frac{\partial^2 C_1}{\partial z^2} - (\alpha_1 + \alpha_{g1}) C_1 \quad (2.26)$$

$$C_1(x, y, z, t) = 0 \quad \text{at} \quad t = 0 \quad (2.27)$$

$$C_1(x, y, z, t) = \frac{Q(t)}{u_1} \delta(y) \delta(z - h_s) \quad \text{at} \quad x = 0 \quad (2.28)$$

$$C_1(x, y, z, t) = 0 \quad \text{as} \quad y \rightarrow \pm \infty \quad (2.29)$$

$$\frac{\partial C_1}{\partial z} = N_1 C_1 \quad \text{at} \quad z = 0 \quad (2.30)$$

$$\frac{\partial C_1}{\partial z} = -L_1 C_1 \quad \text{at} \quad z = 1 \quad (2.31)$$

$$\frac{\partial C_{p1}}{\partial t} + u_1 \frac{\partial C_{p1}}{\partial x} = \beta_1 \frac{\partial^2 C_{p1}}{\partial y^2} + \gamma_1 \frac{\partial^2 C_{p1}}{\partial z^2} + \alpha_1 C_1 - \alpha_{p1} C_{p1} \quad (2.32)$$

$$C_{p1}(x, y, z, t) = 0 \quad \text{at} \quad t = 0 \quad (2.33)$$

$$C_{p1}(x, y, z, t) = 0 \quad \text{at} \quad x = 0; y = 0, z = h_s \quad (2.34)$$

$$C_{p1}(x, y, z, t) = 0 \quad \text{as} \quad y \rightarrow \pm \infty \quad (2.35)$$

$$\frac{\partial C_{p1}}{\partial z} = N_{p1} C_{p1} \quad \text{at} \quad z = 0 \quad (2.36)$$

$$\frac{\partial C_{p1}}{\partial z} = -L_{p1} C_{p1} \quad \text{at} \quad z = 1 \quad (2.37)$$

Patch II  $(x \geq x_1, 0 \leq z \leq 1)$

$$\frac{\partial C_2}{\partial t} + u_2 \frac{\partial C_2}{\partial x} = \beta_2 \frac{\partial^2 C_2}{\partial y^2} + \gamma_2 \frac{\partial^2 C_2}{\partial z^2} - (\alpha_2 + \alpha_{g2} + \delta_1) C_2 \quad (2.38)$$

$$C_2(x, y, z, t) = 0 \quad \text{at} \quad t = 0 \quad (2.39)$$

$$C_2(x, y, z, t) = C_1(x, y, z, t) \quad \text{at} \quad x = x_1 \quad (2.40)$$

$$C_2(x, y, z, t) = 0 \quad \text{as} \quad y \rightarrow \pm \infty \quad (2.41)$$



$$\frac{\partial C_2}{\partial z} = N_2 C_2 \quad \text{at } z = 0 \quad (2.42)$$

$$\frac{\partial C_2}{\partial z} = -L_2 C_2 \quad \text{at } z = 1 \quad (2.43)$$

$$\frac{\partial C_{p2}}{\partial t} + u_2 \frac{\partial C_{p2}}{\partial x} = \beta_2 \frac{\partial^2 C_{p2}}{\partial y^2} + \gamma_2 \frac{\partial^2 C_{p2}}{\partial z^2} + \alpha_2 C_2 - (\alpha_{p2} + \delta_2) C_{p2} \quad (2.44)$$

$$C_{p2}(x, y, z, t) = 0 \quad \text{at } t = 0 \quad (2.45)$$

$$C_{p2}(x, y, z, t) = C_{p1}(x, y, z, t) \quad \text{at } x = x_1 \quad (2.46)$$

$$C_{p2}(x, y, z, t) = 0 \quad \text{as } y \rightarrow \pm \infty \quad (2.47)$$

$$\frac{\partial C_{p2}}{\partial z} = N_{p2} C_{p2} \quad \text{at } z = 0 \quad (2.48)$$

$$\frac{\partial C_{p2}}{\partial z} = -L_{p2} C_{p2} \quad \text{at } z = 1 \quad (2.49)$$

where

$$\begin{aligned} \alpha_i &= \frac{k_i H^2}{K_{z0}}, & \beta_i &= \frac{K_{yi}}{K_{z0}}, & \gamma_i &= \frac{K_{zi}}{K_{z0}}, & \alpha_{pi} &= \frac{k_{pi} H^2}{K_{z0}}, \\ \alpha_{gi} &= \frac{k_{gi} H^2}{K_{z0}}, & N_i &= \frac{v_{di} H}{K_{zi}}, & N_{pi} &= \frac{v_{dpi} H}{K_{zi}}, & L_i &= \frac{w_i H}{K_{zi}}, \\ L_{pi} &= \frac{w_{pi} H}{K_{zi}}, \quad i = 1, 2 \end{aligned}$$

$$(i) \quad Q(t) = Q_0 \delta(t)$$

$$(ii) \quad Q(t) = 1 \quad (2.50)$$

$$\begin{aligned} (iii) \quad Q(t) &= 1, & 0 \leq t \leq t_0 \\ &= 0, & t > t_0 \end{aligned}$$

## 2.2 METHOD OF SOLUTION

Following Astarita *et al.*(1979), Alam and Seinfeld(1981), equations (2.26) and (2.32) can be written in compact form as,

$$\mathcal{L}_1 \begin{bmatrix} C_1 \\ C_{p1} \end{bmatrix} - \begin{bmatrix} \alpha_1 + \alpha_{g1} & 0 \\ -\alpha_1 & \alpha_{p1} \end{bmatrix} \begin{bmatrix} C_1 \\ C_{p1} \end{bmatrix} = 0 \quad (2.51)$$

where  $\mathcal{L}_1$  is the advection/diffusion operator

$$\mathcal{L}_1 \equiv -\frac{\partial}{\partial t} - u_1 \frac{\partial}{\partial x} + \beta_1 \frac{\partial^2}{\partial y^2} + \gamma_1 \frac{\partial^2}{\partial z^2}$$

To uncouple this system, we define a matrix,

$$A_1 = \begin{bmatrix} \alpha_1 + \alpha_{g1} & 0 \\ -\alpha_1 & \alpha_{p1} \end{bmatrix}$$

which can be written as  $A_1 = M_1 R M_1^{-1}$ , where

$$M_1 = \begin{bmatrix} 1 & 0 \\ \frac{\alpha_1}{\alpha_{p1} - \alpha_1 - \alpha_{g1}} & 1 \end{bmatrix} \quad R = \begin{bmatrix} \alpha_1 + \alpha_{g1} & 0 \\ 0 & \alpha_{p1} \end{bmatrix}$$

$$M_1^{-1} = \begin{bmatrix} 1 & 0 \\ -\alpha_1 & 1 \\ \frac{\alpha_{p1} - \alpha_1 - \alpha_{g1}}{\alpha_1} & \end{bmatrix}$$

If we define a new concentration  $B_1$  such that

$$\begin{bmatrix} C_1 \\ B_1 \end{bmatrix} = M_1^{-1} \begin{bmatrix} C_1 \\ C_{p1} \end{bmatrix}$$

the uncoupled system for patch I can be written as,

$$\mathcal{L}_1 C_1 - (\alpha_1 + \alpha_{g1}) C_1 = 0 \quad (2.52)$$

$$\mathcal{L}_1 B_1 - \alpha_{p1} B_1 = 0 \quad (2.53)$$

$$\text{where } B_1 = C_{p1} - \frac{\alpha_1}{\alpha_{p1} - \alpha_1 - \alpha_{g1}} C_1 \quad (2.54)$$

The conditions for  $C_1$  remains same. The corresponding conditions for  $B_1$  are,

$$B_1(x, y, z, t) = 0 \quad \text{at } t = 0 \quad (2.55)$$

$$B_1(x, y, z, t) = - \frac{\alpha_1}{\alpha_{p1} - \alpha_1 - \alpha_{g1}} \frac{Q(t)}{u_1} \delta(y) \delta(z-h_s) \quad \text{at } x = 0 \quad (2.56)$$

$$B_1(x, y, z, t) = 0 \quad \text{as } y \rightarrow \pm \infty \quad (2.57)$$

$$\frac{\partial B_1}{\partial z} = N_{p1} B_1 + \frac{N_{p1} - N_1}{\alpha_{p1} - \alpha_1 - \alpha_{g1}} \alpha_1 C_1 \quad \text{at } z = 0 \quad (2.58)$$

$$\frac{\partial B_1}{\partial z} = -L_{p1} B_1 + \frac{L_1 - L_{p1}}{\alpha_{p1} - \alpha_1 - \alpha_{g1}} \alpha_1 C_1 \quad \text{at } z = 1 \quad (2.59)$$

Similarly we also get uncoupled system for Patch-II corresponding to equations (2.38) and (2.44),

$$\mathcal{L}_2 C_2 - (\alpha_2 + \alpha_{g2} + \delta_1) C_2 = 0 \quad (2.60)$$

$$\mathcal{L}_2 B_2 - (\alpha_{p2} + \delta_2) B_2 = 0 \quad (2.61)$$

$$\text{where } \mathcal{L}_2 = - \frac{\partial}{\partial t} - u_2 \frac{\partial}{\partial x} + \beta_2 \frac{\partial^2}{\partial y^2} + \gamma_2 \frac{\partial^2}{\partial z^2} \quad (2.62)$$

$$\text{and } B_2 = C_{p2} - \frac{\alpha_2}{\alpha_{p2} - \alpha_2 - \alpha_{g2} + \delta_2 - \delta_1} C_2 \quad (2.63)$$

The conditions for  $C_2$  remains same. The corresponding conditions for  $B_2$  are,

$$B_2(x, y, z, t) = 0 \quad \text{at } t = 0 \quad (2.64)$$

$$B_2(x, y, z, t) = B_1(x, y, z, t) + \left( \frac{\alpha_1}{\alpha_{p1} - \alpha_1 - \alpha_{g1}} - \frac{\alpha_2}{\alpha_{p2} - \alpha_2 - \alpha_{g2} + \delta_2 - \delta_1} \right) C_1 \quad \text{at } x = x_1 \quad (2.65)$$

$$B_2(x, y, z, t) = 0 \quad \text{as } y \rightarrow \pm \infty \quad (2.66)$$

$$\frac{\partial B_2}{\partial z} = N_{p2} B_2 + \frac{N_{p2} - N_2}{\alpha_{p2} - \alpha_2 - \alpha_{g2} + \delta_2 - \delta_1} \alpha_2 C_2 \quad \text{at } z = 0 \quad (2.67)$$

$$\frac{\partial B_2}{\partial z} = -L_{p2} B_2 + \frac{L_2 - L_{p2}}{\alpha_{p2} - \alpha_2 - \alpha_{g2} + \delta_2 - \delta_1} \alpha_2 C_2 \quad \text{at } z = 1 \quad (2.68)$$

### 2.3 CONCENTRATION DISTRIBUTIONS

The solutions for  $C_1$ ,  $B_1$  and  $C_2$ ,  $B_2$  are obtained using Laplace and Fourier transform techniques, (Carslaw and Jaeger, 1959) in each cases as,

#### 2.3.1 CASE I WHEN FLUX IS INSTANTANEOUS AT THE SOURCE

$$Q(t) = Q_0 \delta(t)$$

$$C_1(x, y, z, t) = \frac{Q_0}{u_1} P(x, y, z) \delta\left(t - \frac{x}{u_1}\right) \quad (2.69)$$

$$B_1(x, y, z, t) = \frac{Q_0}{u_1} Q(x, y, z) \delta\left(t - \frac{x}{u_1}\right) \quad (2.70)$$

$$C_2(x, y, z, t) = \frac{Q_0}{u_1} M(x, y, z) \delta\left(t - \left(\frac{x_1}{u_1} + \frac{x-x_1}{u_2}\right)\right) \quad (2.71)$$

$$B_2(x, y, z, t) = \frac{Q_0}{u_1} N(x, y, z) \delta\left(t - \left(\frac{x_1}{u_1} + \frac{x-x_1}{u_2}\right)\right) \quad (2.72)$$

where

$$P(x, y, z) = \frac{e^{-y^2/(4\frac{\beta_1}{u_1}x)}}{\sqrt{4\pi \frac{\beta_1}{u_1} x}} \sum_{n=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \alpha_{g1} + \gamma_1 \lambda_n^2}{u_1}\right)x\right) \frac{F_n(h_s)}{P_n} F_n(z)$$

$$Q(x, y, z) = \frac{e^{-y^2/(4\frac{\beta_1}{u_1}x)}}{\sqrt{4\pi \frac{\beta_1}{u_1} x}} \sum_{n=1}^{\infty} \frac{\alpha_1}{\alpha_{p1} - \alpha_1 - \alpha_{g1}} \exp\left(-\left(\frac{\alpha_{p1} + \gamma_1 \xi_n^2}{u_1}\right)x\right) \frac{H_n(z)}{P_{n1}}$$

$$\left( \sum_{m=1}^{\infty} \frac{\gamma_1}{u_1} \xi_n^2 \frac{F_m(h_s)}{P_m} I_{11} I_{12} - H_n(h_s) \right)$$

$$M(x, y, z) = \frac{e^{-y^2/4\beta(x)}}{\sqrt{4\pi\beta(x)}} \sum_{n=1}^{\infty} \exp\left(-\left(\frac{\alpha_2 + \alpha_{g2} + \delta_1 + \gamma_2 \mu_n^2}{u_2}\right)(x - x_1)\right) \frac{G_n(z)}{Q_n}$$

$$\sum_{m=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \alpha_{g1} + \gamma_1 \lambda_m^2}{u_1}\right)x_1\right) \frac{F_m(h_s)}{P_m} \int_0^1 F_m(z) G_n(z) dz$$

$$N(x, y, z) = \frac{e^{-y^2/4\beta(x)}}{\sqrt{4\pi\beta(x)}} \sum_{n=1}^{\infty} \exp\left(-\left(\frac{\alpha_{p2} + \delta_2 + \gamma_2 \nu_n^2}{u_2}\right)(x - x_1)\right) \frac{J_n(z)}{P_{n2}}$$

$$\left[ \sum_{r=1}^{\infty} \frac{a_{11}}{P_{r1}} \exp\left(-\left(\frac{\alpha_{p1} + \gamma_1 \xi_r^2}{u_1}\right)x_1\right) \int_0^1 H_r(z) J_n(z) dz \left\{ \sum_{m=1}^{\infty} \frac{\gamma_1}{u_1} \xi_r^2 \frac{F_m(h_s)}{P_m} \right. \right.$$

$$I_{21} I_{22} - H_r(h_s) \left. \right\} + \sum_{r=1}^{\infty} (a_{11} - a_{12}) \exp\left(-\left(\frac{\alpha_1 + \alpha_{g1} + \gamma_1 \lambda_r^2}{u_1}\right)x_1\right) \frac{F_r(h_s)}{P_r}$$

$$\int_0^1 F_r(z) J_n(z) dz + \sum_{r=1}^{\infty} \frac{a_{12}}{Q_r} \frac{\gamma_2}{u_2} \nu_n^2 I_{23} I_{24} \sum_{m=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \alpha_{g1} + \gamma_1 \lambda_m^2}{u_1}\right)x_1\right)$$

$$\left[ \frac{F_m(h_s)}{P_m} \int_0^1 F_m(z) G_r(z) dz \right]$$

$$F_n(z) = \cos \lambda_n z + \frac{N_1}{\lambda_n} \sin \lambda_n z$$

$$G_n(z) = \cos \mu_n z + \frac{N_2}{\mu_n} \sin \mu_n z$$

$$H_n(z) = \cos \xi_n z + \frac{N_{p1}}{\xi_n} \sin \xi_n z$$

$$J_n(z) = \cos \nu_n z + \frac{N_{p2}}{\nu_n} \sin \nu_n z$$

$$P_n = \int_0^1 (\cos \lambda_n z + \frac{N_1}{\lambda_n} \sin \lambda_n z)^2 dz$$

$$Q_n = \int_0^1 (\cos \mu_n z + \frac{N_2}{\mu_n} \sin \mu_n z)^2 dz$$

$$P_{n1} = \int_0^1 (\cos \xi_n z + \frac{N_{p1}}{\xi_n} \sin \xi_n z)^2 dz$$

$$P_{n2} = \int_0^1 (\cos \nu_n z + \frac{N_{p2}}{\nu_n} \sin \nu_n z)^2 dz$$

Here  $\lambda_n$ ,  $\mu_n$ ,  $\xi_n$  and  $\nu_n$  are the roots of the following transcendental equations,

$$\tan \lambda_n = \frac{\lambda_n (L_1 + N_1)}{\lambda_n^2 - L_1 N_1}, \quad n = 1, 2, \dots$$

$$\tan \mu_n = \frac{\mu_n (L_2 + N_2)}{\mu_n^2 - L_2 N_2}$$

$$\tan \xi_n = \frac{\xi_n (L_{p1} + N_{p1})}{\xi_n^2 - L_{p1} N_{p1}}$$

$$\tan \nu_n = \frac{\nu_n (L_{p2} + N_{p2})}{\nu_n^2 - L_{p2} N_{p2}}$$

$$I_{11} = \int_0^1 (a_{2m} z + a_{4m}) H_n(z) dz$$

$$I_{12} = \int_0^x \exp \left( - \left( \frac{\alpha_1 + \alpha_{g1} - \alpha_{p1} + \gamma_1 \lambda_m^2 - \gamma_1 \xi_n^2}{u_1} \right) x' \right) dx'$$

$$I_{21} = \int_0^1 (a_{2m} z + a_{4m}) H_r(z) dz$$

$$I_{22} = \int_0^{x_1} \exp \left( - \left( \frac{\alpha_1 + \alpha_{g1} - \alpha_{p1} + \gamma_1 \lambda_m^2 - \gamma_1 \xi_r^2}{u_1} \right) x' \right) dx'$$

$$I_{23} = \int_0^1 (a_{6r} z + a_{7r}) J_n(z) dz$$

$$I_{24} = \int_0^{x-x_1} \exp \left( - \left( \frac{\alpha_2 + \alpha_{g2} + \delta_1 + \gamma_2 \mu_r^2 - \gamma_2 \nu_n^2 - \alpha_{p2} - \delta_2}{u_2} \right) x' \right) dx'$$

$$a_{11} = \frac{\alpha_1}{\alpha_{p1} - \alpha_1 - \alpha_{g1}}$$

$$a_{12} = \frac{\alpha_2}{\alpha_{p2} + \delta_2 - \alpha_2 - \alpha_{g2} - \delta_1}$$

$$a_{2n} = \frac{(N_{p1} - N_1) L_{p1} + (L_1 - L_{p1}) N_{p1} F_n(1)}{L_{p1} + (1 + L_{p1}) N_{p1}}$$

$$a_{4n} = \frac{a_{2n}}{N_{p1}} - \frac{N_{p1} - N_1}{N_{p1}}$$

$$\beta(x) = \frac{\beta_1}{u_1} x_1 + \frac{\beta_2}{u_2} (x - x_1)$$

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$$a_{6n} = \frac{(N_{p2} - N_2) L_{p2} + (L_2 - L_{p2}) G_n(1) N_{p2}}{L_{p2} + (1 + L_{p2}) N_{p2}}$$

$$a_{7n} = \frac{a_{6n}}{N_{p2}} - \frac{N_{p2} - N_2}{N_{p2}}$$

and  $\delta(t-x)$  is the Dirac delta function defined as, (Carslaw and Jaeger, 1941)

$$\begin{aligned}\delta(t-x) &= 0, \quad t < x \\ &= \frac{1}{\epsilon}, \quad x \leq t \leq x + \epsilon \\ &= 0, \quad t > x + \epsilon\end{aligned}$$

### 2.3.2 CASE II WHEN FLUX IS CONSTANT AT THE SOURCE $Q(t) = 1$

$$C_1(x, y, z, t) = \frac{1}{u_1} P(x, y, z) H\left(t - \frac{x}{u_1}\right) \quad (2.73)$$

$$B_1(x, y, z, t) = \frac{1}{u_1} Q(x, y, z) H\left(t - \frac{x}{u_1}\right) \quad (2.74)$$

$$C_2(x, y, z, t) = \frac{1}{u_1} M(x, y, z) H\left(t - \left(\frac{x_1}{u_1} + \frac{x-x_1}{u_2}\right)\right) \quad (2.75)$$

$$B_2(x, y, z, t) = \frac{1}{u_1} N(x, y, z) H\left(t - \left(\frac{x_1}{u_1} + \frac{x-x_1}{u_2}\right)\right) \quad (2.76)$$

where  $H(t-x)$  is the Heaviside function defined as, (Carslaw and Jaeger, 1941)

$$\begin{aligned}H(t-x) &= 0, \quad t \leq x \\ &= \frac{t}{x+\epsilon}, \quad x < t < x + \epsilon \\ &= 1, \quad t \geq x + \epsilon\end{aligned}$$

From equations (2.73) - (2.76) it is observed that if  $t \rightarrow \infty$  the expressions reduce to the case of steady state. It may also be noted that when  $t < x/u_1$ , the concentration of pollutants is zero i.e., the pollutant front has not reached that point. Also from equations (2.73) and (2.74) it is noted that if  $L_1$  and  $L_{p1}$  are



zero i.e., if there is no leakage into the inversion base and  $t \rightarrow \infty$ , the solutions for  $C_1$  and  $B_1$  reduce to the same form of steady state solutions as obtained by Alam and Seinfeld(1981).

### 2.3.3 CASE III WHEN FLUX IS STEP FUNCTION TYPE AT THE SOURCE

$$Q(t) = 1, \quad 0 \leq t \leq t_0$$

$$= 0, \quad t > t_0$$

$$C_1(x, y, z, t) = \frac{1}{u_1} P(x, y, z) \left[ H\left(t - \frac{x}{u_1}\right) - H\left(t - t_0 - \frac{x}{u_1}\right) H(t - t_0) \right] \quad (2.77)$$

$$B_1(x, y, z, t) = \frac{1}{u_1} Q(x, y, z) \left[ H\left(t - \frac{x}{u_1}\right) - H\left(t - t_0 - \frac{x}{u_1}\right) H(t - t_0) \right] \quad (2.78)$$

$$C_2(x, y, z, t) = \frac{1}{u_1} M(x, y, z) \left[ H\left(t - \left(\frac{x_1}{u_1} + \frac{x - x_1}{u_2}\right)\right) - H\left(t - t_0 - \left(\frac{x_1}{u_1} + \frac{x - x_1}{u_2}\right)\right) H(t - t_0) \right] \quad (2.79)$$

$$B_2(x, y, z, t) = \frac{1}{u_1} N(x, y, z) \left[ H\left(t - \left(\frac{x_1}{u_1} + \frac{x - x_1}{u_2}\right)\right) - H\left(t - t_0 - \left(\frac{x_1}{u_1} + \frac{x - x_1}{u_2}\right)\right) H(t - t_0) \right] \quad (2.80)$$

From equations (2.77)-(2.80) it is seen that as  $t_0 \rightarrow \infty$ , these equations reduce to equations (2.73)-(2.76) respectively.

The concentrations  $C_{p1}$  and  $C_{p2}$  can now be obtained from  $C_1$ ,  $B_1$  and  $C_2$ ,  $B_2$  in each of the above cases by the following relations,

$$C_{p1}(x, y, z, t) = B_1(x, y, z, t) + \frac{\alpha_1}{\alpha_{p1} - \alpha_1 - \alpha_{g1}} C_1(x, y, z, t)$$

$$C_{p2}(x,y,z,t) = B_2(x,y,z,t) + \frac{\alpha_2}{\alpha_{p2} - \alpha_2 - \alpha_{g2} + \delta_2 - \delta_1} C_2(x,y,z,t)$$

It may be noted here that the solutions above are written in terms of integrals for brevity only although these can be evaluated in exact forms which are very lengthy to write.

## 2.4 DISCUSSION AND RESULTS

To see the effects of removal parameters, the expressions for concentration distribution of both primary and secondary pollutants in both the patches have been computed and displayed graphically in Figures 2.2-2.8. The parameter values used in the computation are taken as (Alam and Seinfeld, 1981):  $k_i = 0.05 \text{ hr}^{-1}$ ,  $k_{gi} = 10^{-5} \text{ sec}^{-1}$ ,  $k_{pi} = 10^{-4} \text{ sec}^{-1}$ ,  $K_{zi} = 5 \text{ m}^2 \text{ sec}^{-1}$ ,  $u_i = 2.25 \text{ m sec}^{-1}$ ,  $w_i = 0.1 \text{ cm sec}^{-1}$ ,  $w_{pi} = 0.01 \text{ cm sec}^{-1}$ , ( $i=1,2$ ),  $v_{d1} = 1.05 \text{ cm sec}^{-1}$ ,  $v_{d2} = 1.0 \text{ cm sec}^{-1}$ ,  $v_{dp1} = 0.105 \text{ cm sec}^{-1}$ ,  $v_{dp2} = 0.10 \text{ cm sec}^{-1}$ ,  $h_s = 200 \text{ m}$ ,  $H = 10^3 \text{ m}$ . The corresponding dimensionless values are found as  $\alpha_i = 2.77$ ,  $\alpha_{gi} = 2.0$ ,  $\alpha_{pi} = 20.0$ ,  $L_i = 0.2$ ,  $L_{pi} = 0.02$ ,  $u_i = 1.0$ ,  $N_1 = 2.1$ ,  $N_2 = 2.0$ ,  $N_{p1} = 0.21$ ,  $N_{p2} = 0.20$ ,  $h_s = 0.20$ ,  $\beta_i = 10.0$ ,  $\gamma_i = 1.0$  and  $x_1 = 0.03$ ,  $y = 0.0$ ,  $\epsilon = 0.005$ .

From the figures it is observed that the concentrations of both primary and secondary pollutants decrease as downwind distance increases in all the three cases. Also the concentration of primary pollutant decreases but that of secondary pollutant increases in all the cases at a particular time and location as the rates of conversion of primary pollutant to secondary pollutant i.e.,  $\alpha_1$  and  $\alpha_2$  in the two patches increase. The effect of removal is, however, to decrease the concentrations of both the species in all the three cases.

When flux is instantaneous at the source, the central line concentrations ( $z = h_s$ ,  $y = 0.0$ ) of both primary and secondary pollutants are plotted in Figures 2.2-2.3 for different values of  $t$ . It is noted that as time increases the concentration of both primary and secondary pollutants decreases. Comparing Figures 2.2 and 2.3 it is seen that the concentration of both the pollutants reduced considerably as removal parameter, associated with the uniformly distributed sink phase, increases.

When flux is constant at the source, the central line concentrations of both the pollutants are shown in Figures 2.4-2.5 for different values of  $t$ . From these figures it is concluded that the concentration of both the pollutants increases as time increases and reaches their respective steady state values as  $t \rightarrow \infty$ . Due to the presence of sink phase the concentration of both the pollutants reduced considerably (compare Figures 2.4 and 2.5 for  $\delta_1 = \delta_2 = 0$ ,  $\delta_1 = \delta_2 = 50$  respectively).

When flux is step function type at the source, the central line concentrations of both the pollutants decrease as time increases for  $t > t_0$  and the behavior is similar to the case of constant flux for  $t \leq t_0$  (see Figures 2.6-2.7). Note that concentrations of both the pollutants have decreased significantly due to presence of sinks.

The effect of variation of removal parameter associated with sink phase with vertical concentration profiles is shown in Figure 2.8. It is observed from this figure that the concentrations of both primary and secondary pollutants decrease as removal parameter increases.

Finally, from the above discussion it may be concluded that the presence of sink phase in the second patch in the form of rain droplets, fog droplets or even externally introduced species (liquid or gas) can be very effective in removing the pollutants from the atmosphere. This analysis thus suggests a mechanism by which toxic gases leaked out in the atmosphere due to accidental discharge, etc. can be removed by introducing suitable liquid or gaseous phase in the environment using mechanical means. The above analysis can also be utilized for studies related to risk analysis particularly in cases of accidental leakages of pollutants/toxicants in the atmosphere such as MIC leakage in a pesticide plant in Bhopal, India.

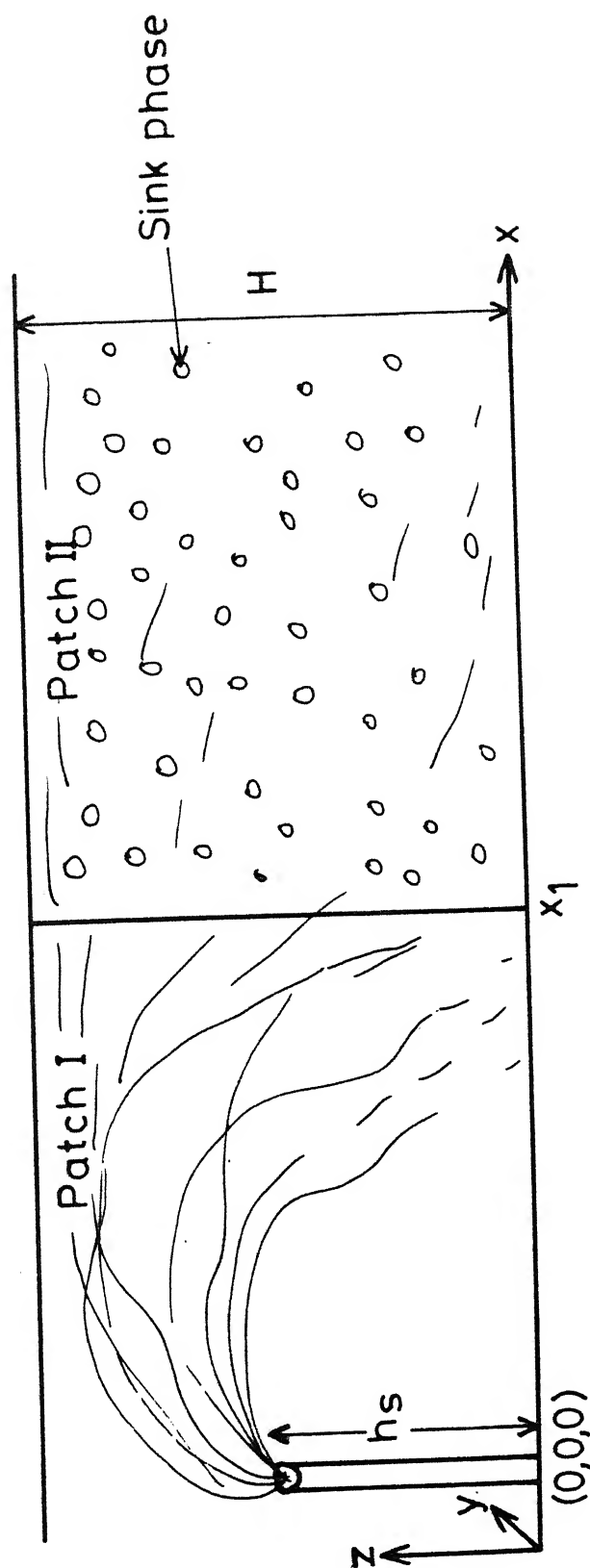


FIG. 2.1 DISPERSION OF AIR POLLUTANT IN A TWO PATCH ENVIRONMENT.

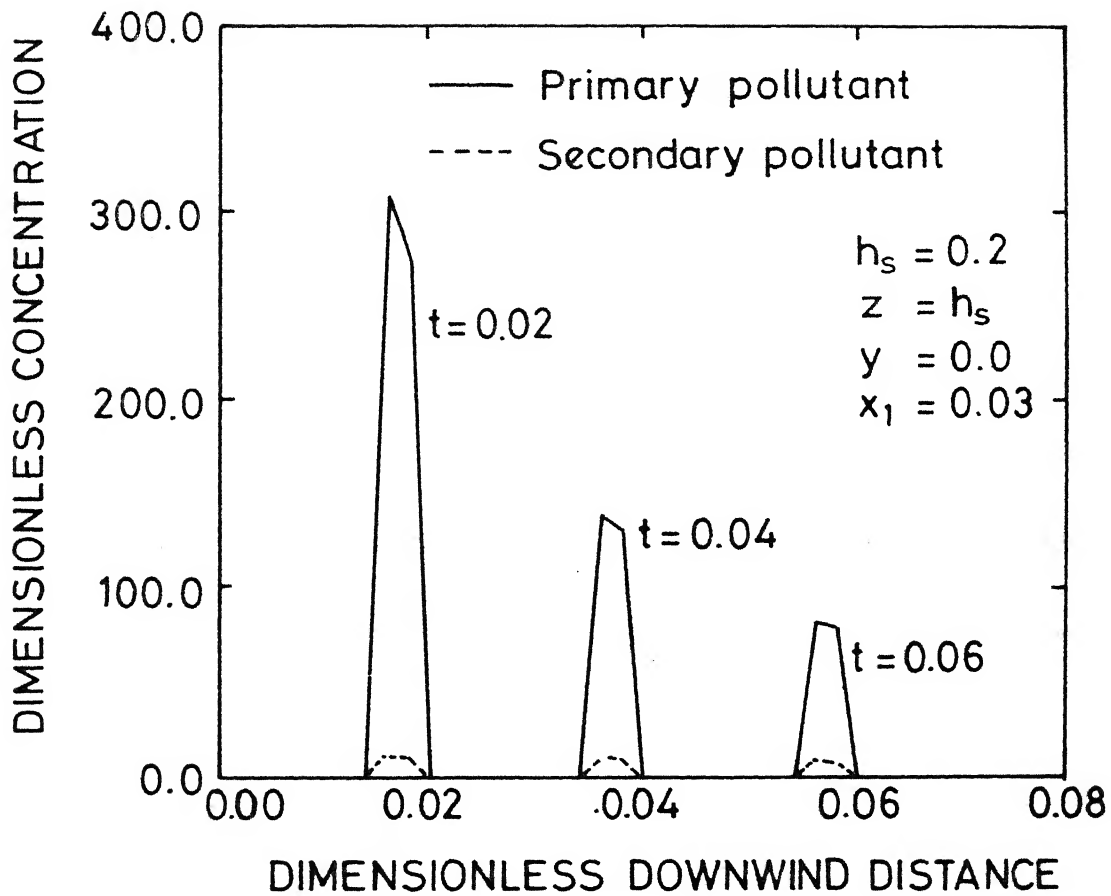


FIG. 2.2 CONCENTRATION-DISTANCE PROFILES FOR INSTANTANEOUS FLUX AT THE SOURCE WITHOUT SINK PHASE,  $\delta_1 = \delta_2 = 0.0$

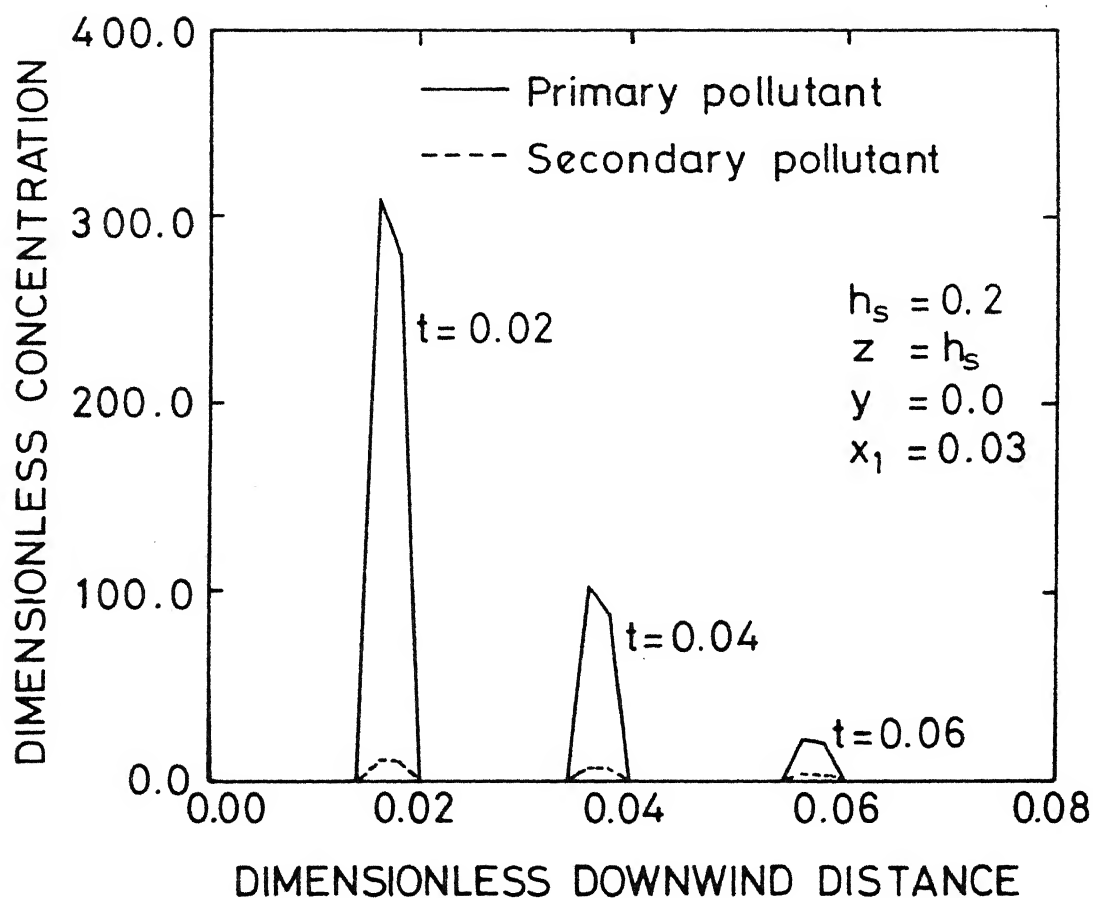


FIG. 2.3 CONCENTRATION-DISTANCE PROFILES FOR INSTANTANEOUS FLUX AT THE SOURCE, WITH SINK PHASE  $\delta_1 = \delta_2 = 50.0$

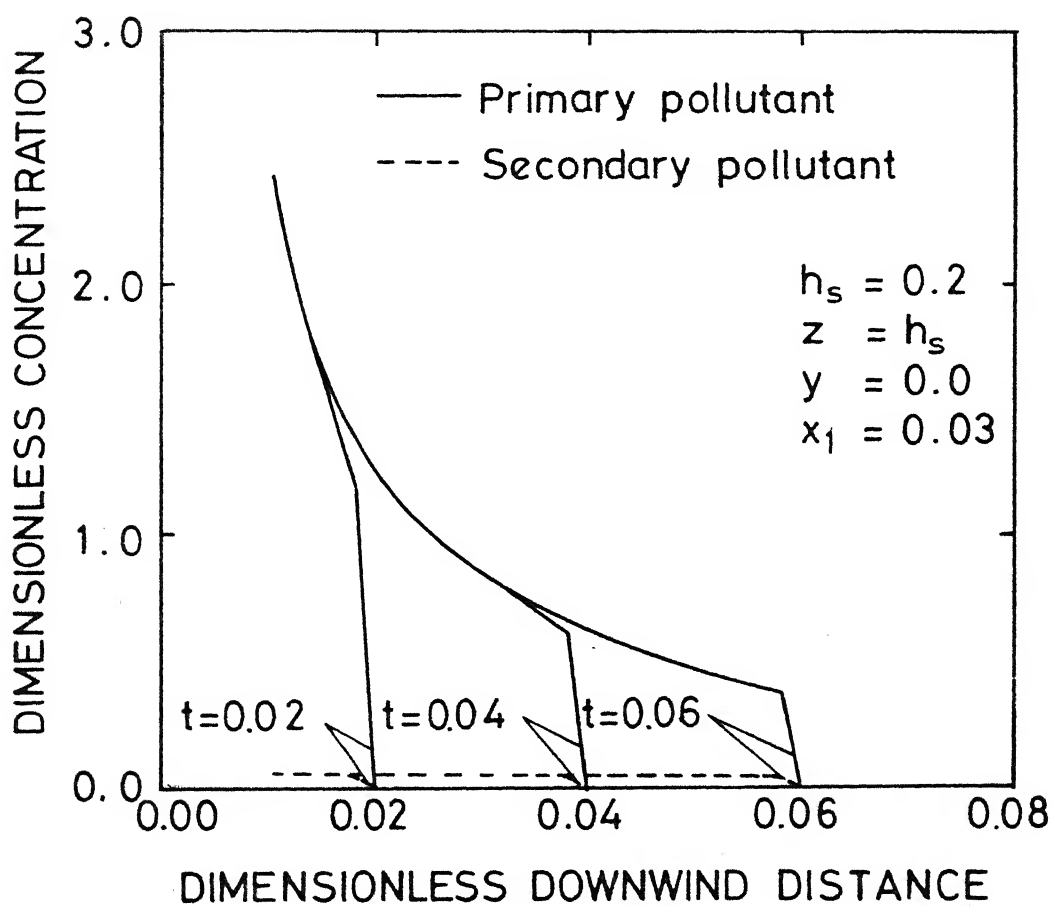


FIG. 2.4 CONCENTRATION-DISTANCE PROFILES FOR CONSTANT FLU AT THE SOURCE, WITHOUT SINK PHASE,  $\delta_1 = \delta_2 = 0.0$



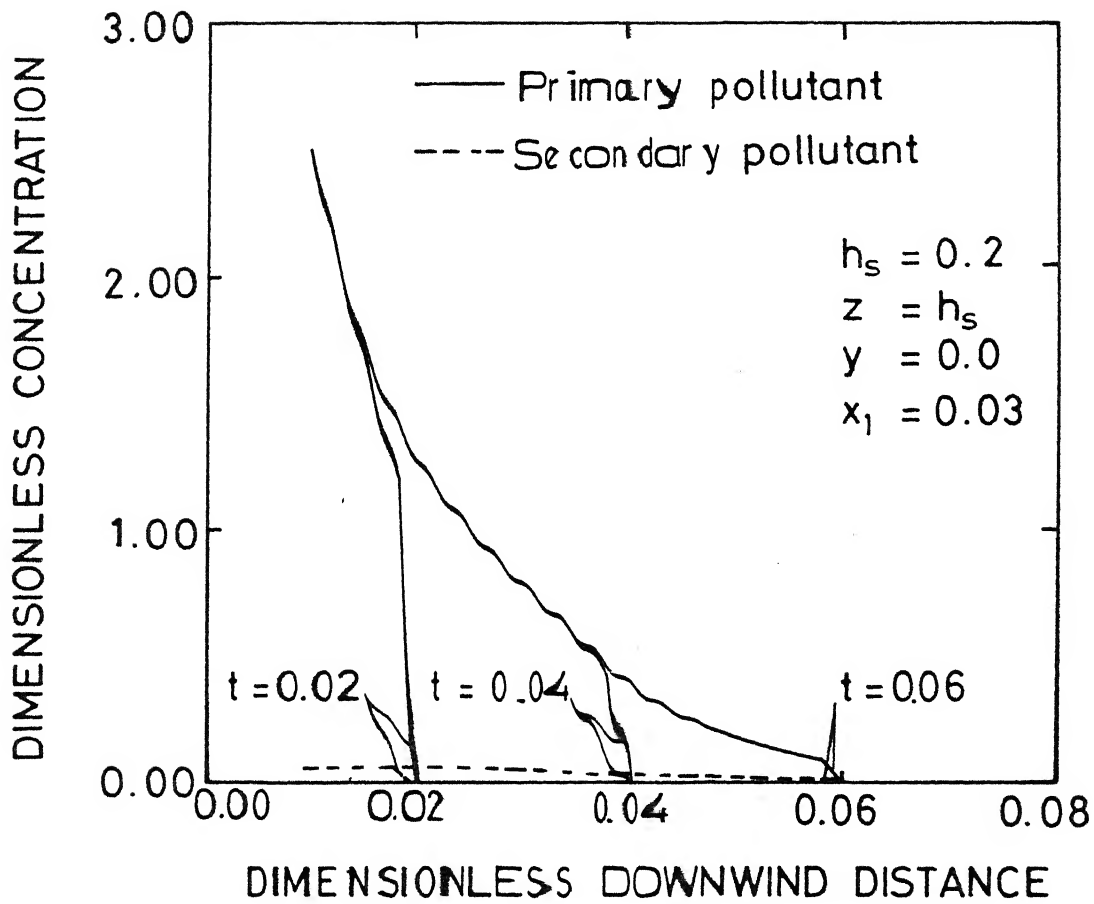


FIG.2.5 CONCENTRATION-DISTANCE PROFILES FOR CONSTANT FLUX AT THE SOURCE, WITH SINK PHASE  $\delta_1 = \delta_2 = 50.0$

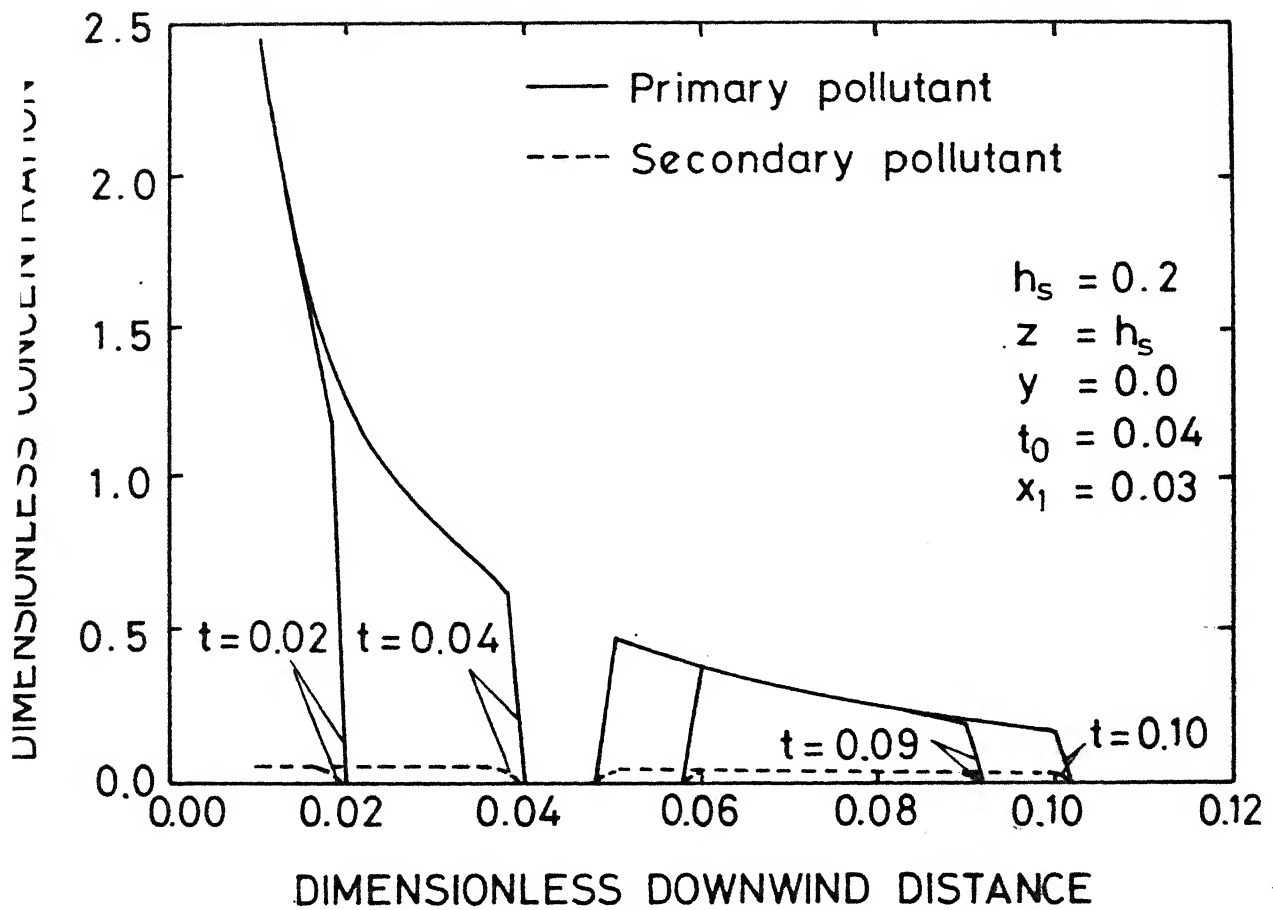


FIG. 2.6 CONCENTRATION-DISTANCE PROFILES FOR STEP FUNCTION TYPE FLUX AT THE SOURCE WITHOUT SINK PHASE,  $\delta_1 = \delta_2 = 0.0$

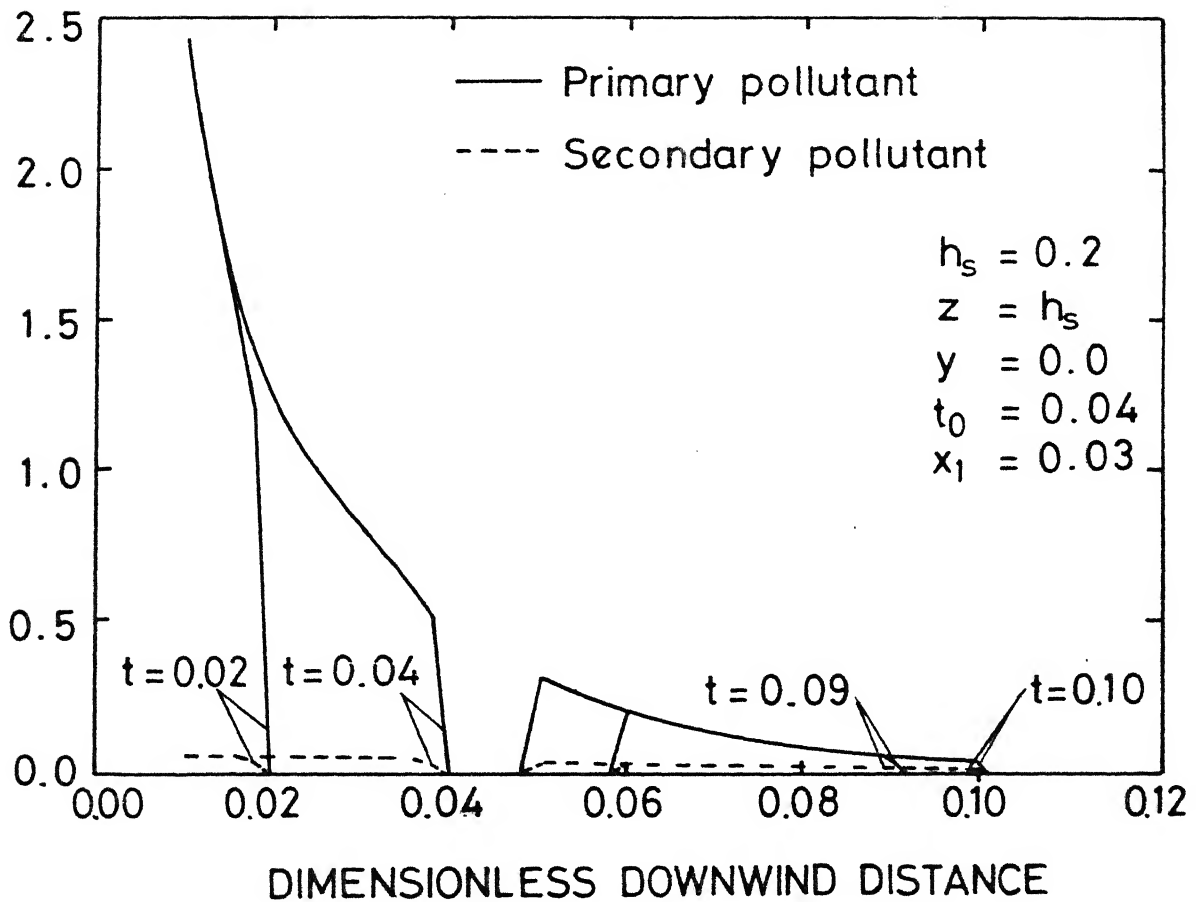


FIG.2.7 CONCENTRATION-DISTANCE PROFILES FOR STEP FUNCTION TYPE FLUX AT THE SOURCE, WITH SINK PHASE,  $\delta_1 = \delta_2 = 20.0$

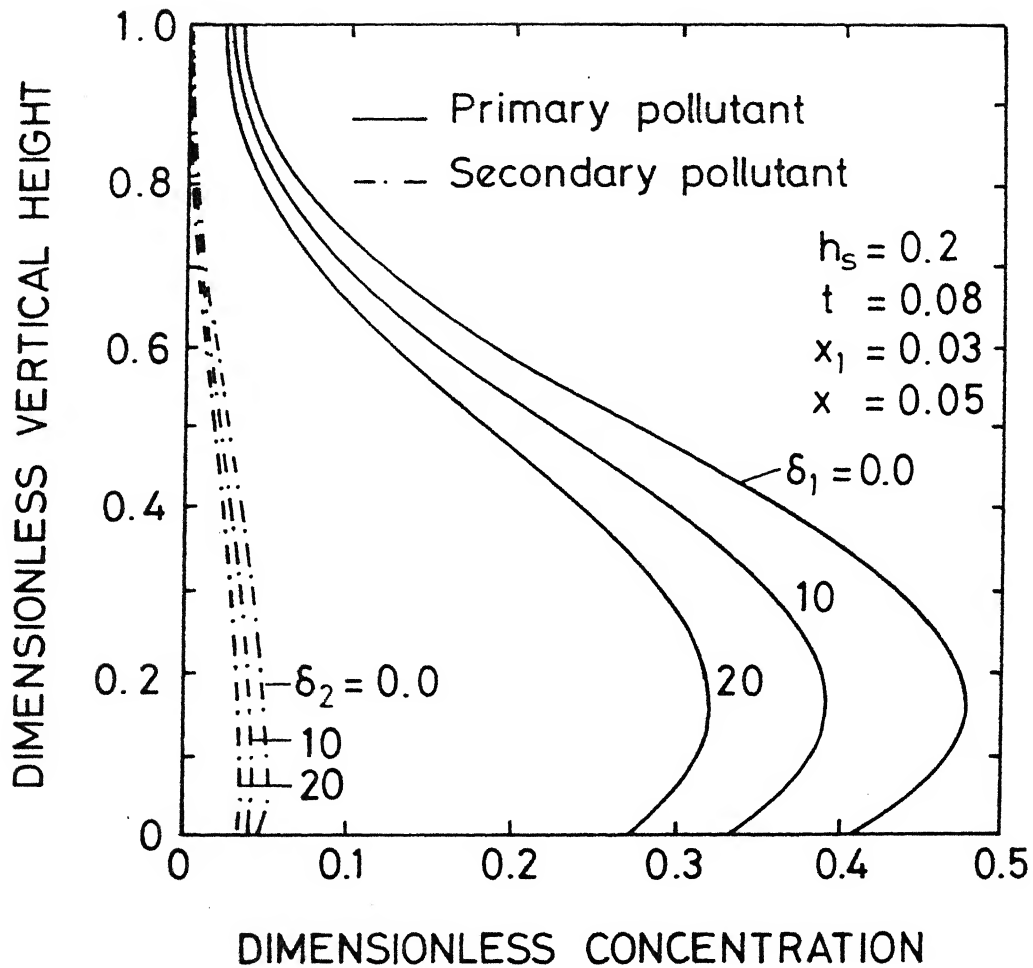


FIG. 2.8 VARIATION OF CONCENTRATION WITH REMOVAL PARAMETER ASSOCIATED WITH SINK PHASE FOR CONSTANT FLUX AT THE SOURCE.

of dust released from an elevated source by taking into account the deposition and settling of dust particles under inversion condition. It may be noted that the sources are, in general, time dependent e.g., accidental explosion of a nuclear device, leakage of toxic material from storage tanks, etc. but very little attention has been paid to study the dispersion in such cases with gravitational settling, Cleary *et al.*(1974), Llewelyn(1983). In particular, Llewelyn(1983) presented the solution of unsteady state three dimensional transport diffusion equation with a first order reaction term for primary pollutant only emitted from a continuous point source using leakage at the base of stable inversion layer and deposition at the ground.

Keeping in view the above, in this chapter we study the unsteady state dispersion of heavier air pollutant emitted from a time dependent point source forming secondary species in a two patch environment to see the effect of gravitational settling, which may be different in the two patches due to formation of fog, etc. The deposition at the ground and first order conversion of primary pollutant to secondary pollutant with removal of both the species has also been taken into account. To do so the unsteady state coupled three dimensional convective diffusion equations involving both primary and secondary pollutants have been solved incorporating the above mentioned factors. As in chapter II the different forms of time dependent flux at the source are considered in the analysis: (i) Instantaneous (ii) Constant, and (iii) Step function type.

### 3.1 MATHEMATICAL MODEL

Consider the unsteady state dispersion of heavier air pollutant, from a time dependent point source of strength  $Q(t)$  located at height  $h_s$  from the ground  $z = 0$ , forming secondary species in a two patch environment under atmospheric inversion as shown in Figure 2.1 of the previous chapter. It is assumed that the time dependent source is located in the first patch and the wind is sufficiently large in both the patches so that downwind diffusion is negligible in comparison to advection.

Under these assumptions the partial differential equations governing the concentration of pollutants in both the patches, with appropriate initial and boundary conditions can be written as follows,

Patch I ( $0 \leq x < x_1$ ,  $0 \leq z \leq H$ )

The differential equation governing the concentration  $C_1(x,y,z,t)$  of the primary pollutant in the first patch is written as,

$$\frac{\partial C_1}{\partial t} + u_1 \frac{\partial C_1}{\partial x} - w_1 \frac{\partial C_1}{\partial z} = K_{y1} \frac{\partial^2 C_1}{\partial y^2} + K_{z1} \frac{\partial^2 C_1}{\partial z^2} - (k_1 + k_{g1})C_1 \quad (3.1)$$

where  $x$ ,  $y$ ,  $z$  are cartesian co-ordinates,  $t$  is the time,  $x$ -axis is taken in the downwind direction and  $z$ -axis vertically upwards,  $u_1$  is the mean wind velocity,  $w_1$  is the settling velocity which, however, depends on the size, shape and weight of the emitted particles but here it is assumed to be independent of position for simplicity, (Fisher and Macqueen, 1977).  $K_{y1}$  and  $K_{z1}$  are diffusivities, assumed to be constants, in  $y$  and  $z$  directions respectively. The constant  $k_1$  is the conversion rate coefficient

of primary pollutant to secondary pollutant and  $k_{g1}$  is its removal rate coefficient.

The initial and boundary conditions for equation (3.1) are,

$$C_1(x, y, z, t) = 0 \quad \text{at } t = 0 \quad (3.2)$$

$$C_1(x, y, z, t) = \frac{Q(t)}{u_1} \delta(y) \delta(z - h_s) \quad \text{at } x = 0 \quad (3.3)$$

$$C_1(x, y, z, t) = 0 \quad \text{as } y \rightarrow \pm \infty \quad (3.4)$$

$$K_{z1} \frac{\partial C_1}{\partial z} + w_1 C_1 = v_{d1} C_1 \quad \text{at } z = 0 \quad (3.5)$$

$$\frac{\partial C_1}{\partial z} = 0 \quad \text{at } z = H \quad (3.6)$$

where  $v_{d1}$  is the deposition velocity of the primary pollutant at the ground  $z = 0$ ,  $H$  is the height of the inversion layer and  $\delta(\cdot)$  is the Dirac delta function.

Similarly the differential equation governing the concentration  $C_{p1}(x, y, z, t)$  of the secondary pollutant can be written as,

$$\frac{\partial C_{p1}}{\partial t} + u_1 \frac{\partial C_{p1}}{\partial x} - w_1 \frac{\partial C_{p1}}{\partial z} = K_{y1} \frac{\partial^2 C_{p1}}{\partial y^2} + K_{z1} \frac{\partial^2 C_{p1}}{\partial z^2} + k_1 C_1 - k_{p1} C_{p1} \quad (3.7)$$

The initial and boundary conditions for equation (3.7) are, (assuming that there is no direct emission of secondary pollutant from the source)

$$C_{p1}(x, y, z, t) = 0 \quad \text{at } t = 0 \quad (3.8)$$

$$C_{p1}(x, y, z, t) = 0 \quad \text{at } x = 0; y = 0, z = h_s \quad (3.9)$$

$$C_{p1}(x, y, z, t) = 0 \quad \text{as } y \rightarrow \pm \infty \quad (3.10)$$

$$K_{z1} \frac{\partial C_{p1}}{\partial z} + w_1 C_{p1} = v_{dp1} C_{p1} \quad \text{at } z = 0 \quad (3.11)$$

$$\frac{\partial C_{p1}}{\partial z} = 0 \quad \text{at } z = H \quad (3.12)$$

where  $v_{dp1}$  is the deposition velocity of the secondary pollutant at  $z = 0$  and  $k_{p1}$  is its removal rate coefficient.

Patch II ( $x \geq x_1$ ,  $0 \leq z \leq H$ )

The differential equation governing the concentration  $C_2(x, y, z, t)$  of the primary pollutant in the second patch is written as,

$$\frac{\partial C_2}{\partial t} + u_2 \frac{\partial C_2}{\partial x} - w_2 \frac{\partial C_2}{\partial z} = K_{y2} \frac{\partial^2 C_2}{\partial y^2} + K_{z2} \frac{\partial^2 C_2}{\partial z^2} - (k_2 + k_{g2}) C_2 \quad (3.13)$$

where  $u_2$  is the mean wind velocity,  $w_2$  is the settling velocity,  $K_{y2}$  and  $K_{z2}$  are diffusivities in  $y$  and  $z$  directions respectively. The constant  $k_2$  is the conversion rate coefficient of primary pollutant to secondary pollutant and  $k_{g2}$  is its removal rate coefficient.

The initial and boundary conditions for equation (3.13) are,

$$C_2(x, y, z, t) = 0 \quad \text{at } t = 0 \quad (3.14)$$

$$C_2(x, y, z, t) = C_1(x, y, z, t) \quad \text{at } x = x_1 \quad (3.15)$$

$$C_2(x, y, z, t) = 0 \quad \text{as } y \rightarrow \pm \infty \quad (3.16)$$

$$K_{z2} \frac{\partial C_2}{\partial z} + w_2 C_2 = v_{d2} C_2 \quad \text{at } z = 0 \quad (3.17)$$

$$\frac{\partial C_2}{\partial z} = 0 \quad \text{at } z = H \quad (3.18)$$

where  $v_{d2}$  is the deposition velocity of the primary pollutant at



$z = 0$ .

Similarly the differential equation governing the concentration  $C_{p2}(x,y,z,t)$  of the secondary pollutant is written as,

$$\frac{\partial C_{p2}}{\partial t} + u_2 \frac{\partial C_{p2}}{\partial x} - w_2 \frac{\partial C_{p2}}{\partial z} = K_{y2} \frac{\partial^2 C_{p2}}{\partial y^2} + K_{z2} \frac{\partial^2 C_{p2}}{\partial z^2} + k_2 C_2 - k_{p2} C_{p2} \quad (3.19)$$

The initial and boundary conditions for equation (3.19) are,

$$C_{p2}(x,y,z,t) = 0 \quad \text{at} \quad t = 0 \quad (3.20)$$

$$C_{p2}(x,y,z,t) = C_{p1}(x,y,z,t) \quad \text{at} \quad x = x_1 \quad (3.21)$$

$$C_{p2}(x,y,z,t) = 0 \quad \text{as} \quad y \rightarrow \pm \infty \quad (3.22)$$

$$K_{z2} \frac{\partial C_{p2}}{\partial z} + w_2 C_{p2} = v_{dp2} C_{p2} \quad \text{at} \quad z = 0 \quad (3.23)$$

$$\frac{\partial C_{p2}}{\partial z} = 0 \quad \text{at} \quad z = H \quad (3.24)$$

where  $v_{dp2}$  is the deposition velocity of the secondary pollutant at  $z = 0$  and  $k_{p2}$  is its removal rate coefficient.

As in the previous chapter, the following forms of flux  $Q(t)$  are considered in the subsequent analysis,

(i) Flux is Instantaneous

$$Q(t) = Q_0 \delta(t)$$

(ii) Flux is Constant (3.25)

$$Q(t) = Q_c$$

(iii) Flux is Step function type

$$Q(t) = Q_c, \quad 0 \leq t \leq t_0 \\ = 0, \quad t > t_0$$

To cast the problem in dimensionless form, the following non-dimensional quantities are defined,

$$\begin{aligned}\bar{t} &= \frac{K_{z0} t}{H^2}, \quad \bar{x} = \frac{K_{z0} x}{u_0 H^2}, \quad \bar{y} = \frac{y}{H}, \quad \bar{z} = \frac{z}{H}, \quad \bar{h}_s = \frac{h_s}{H}, \\ \bar{u}_i &= \frac{u_i}{u_0}, \quad \bar{C}_i = \frac{u_0 H^2}{Q_c} C_i, \quad \bar{C}_{pi} = \frac{u_0 H^2}{Q_c} C_{pi}, \quad \bar{Q}(t) = \frac{Q(t)}{Q_c}, \\ \bar{Q}_0 &= \frac{Q_0}{Q_c} \frac{K_{z0}}{H^2}, \quad \bar{w}_i = \frac{H w_i}{K_{zi}}, \quad i = 1, 2\end{aligned}$$

where  $K_{z0}$  and  $u_0$  are reference diffusion coefficient and wind velocity respectively.

The equations (3.1-3.25) can be written in dimensionless form (dropping bars for convenience) as:

Patch I ( $0 \leq x < x_1$ ,  $0 \leq z \leq 1$ )

$$\frac{\partial C_1}{\partial t} + u_1 \frac{\partial C_1}{\partial x} - w_1 \frac{\partial C_1}{\partial z} = \beta_1 \frac{\partial^2 C_1}{\partial y^2} + \gamma_1 \frac{\partial^2 C_1}{\partial z^2} - (\alpha_1 + \alpha_{g1}) C_1 \quad (3.26)$$

$$C_1(x, y, z, t) = 0 \quad \text{at} \quad t = 0 \quad (3.27)$$

$$C_1(x, y, z, t) = \frac{Q(t)}{u_1} \delta(y) \delta(z - h_s) \quad \text{at} \quad x = 0 \quad (3.28)$$

$$C_1(x, y, z, t) = 0 \quad \text{as} \quad y \rightarrow \pm \infty \quad (3.29)$$

$$\frac{\partial C_1}{\partial z} + w_1 C_1 = N_1 C_1 \quad \text{at} \quad z = 0 \quad (3.30)$$

$$\frac{\partial C_1}{\partial z} = 0 \quad \text{at} \quad z = 1 \quad (3.31)$$

$$\frac{\partial C_{p1}}{\partial t} + u_1 \frac{\partial C_{p1}}{\partial x} - w_1 \frac{\partial C_{p1}}{\partial z} = \beta_1 \frac{\partial^2 C_{p1}}{\partial y^2} + \gamma_1 \frac{\partial^2 C_{p1}}{\partial z^2} + \alpha_1 C_1 - \alpha_{p1} C_{p1} \quad (3.32)$$

$$C_{p1}(x, y, z, t) = 0 \quad \text{at} \quad t = 0 \quad (3.33)$$

$$C_{p1}(x, y, z, t) = 0 \quad \text{at} \quad x = 0; y = 0, z = h_s \quad (3.34)$$

$$C_{p1}(x, y, z, t) = 0 \quad \text{as} \quad y \rightarrow \pm \infty \quad (3.35)$$

$$\frac{\partial C_{p1}}{\partial z} + w_1 C_{p1} = N_{p1} C_{p1} \quad \text{at} \quad z = 0 \quad (3.36)$$

$$\frac{\partial C_{p1}}{\partial z} = 0 \quad \text{at} \quad z = 1 \quad (3.37)$$

Patch II  $(x \geq x_1, 0 \leq z \leq 1)$

$$\frac{\partial C_2}{\partial t} + u_2 \frac{\partial C_2}{\partial x} - w_2 \frac{\partial C_2}{\partial z} = \beta_2 \frac{\partial^2 C_2}{\partial y^2} + \gamma_2 \frac{\partial^2 C_2}{\partial z^2} - (\alpha_2 + \alpha_{g2}) C_2 \quad (3.38)$$

$$C_2(x, y, z, t) = 0 \quad \text{at} \quad t = 0 \quad (3.39)$$

$$C_2(x, y, z, t) = C_1(x, y, z, t) \quad \text{at} \quad x = x_1 \quad (3.40)$$

$$C_2(x, y, z, t) = 0 \quad \text{as} \quad y \rightarrow \pm \infty \quad (3.41)$$

$$\frac{\partial C_2}{\partial z} + w_2 C_2 = N_2 C_2 \quad \text{at} \quad z = 0 \quad (3.42)$$

$$\frac{\partial C_2}{\partial z} = 0 \quad \text{at} \quad z = 1 \quad (3.43)$$

$$\frac{\partial C_{p2}}{\partial t} + u_2 \frac{\partial C_{p2}}{\partial x} - w_2 \frac{\partial C_{p2}}{\partial z} = \beta_2 \frac{\partial^2 C_{p2}}{\partial y^2} + \gamma_2 \frac{\partial^2 C_{p2}}{\partial z^2} + \alpha_2 C_2 - \alpha_{p2} C_{p2} \quad (3.44)$$

$$C_{p2}(x, y, z, t) = 0 \quad \text{at} \quad t = 0 \quad (3.45)$$

$$C_{p2}(x, y, z, t) = C_{p1}(x, y, z, t) \quad \text{at} \quad x = x_1 \quad (3.46)$$

$$C_{p2}(x, y, z, t) = 0 \quad \text{as} \quad y \rightarrow \pm \infty \quad (3.47)$$

$$\frac{\partial C_{p2}}{\partial z} + w_2 C_{p2} = N_{p2} C_{p2} \quad \text{at } z = 0 \quad (3.48)$$

$$\frac{\partial C_{p2}}{\partial z} = 0 \quad \text{at } z = 1 \quad (3.49)$$

$$\text{where } \alpha_i = \frac{k_i H^2}{K_{z0}}, \quad \beta_i = \frac{K_{yi}}{K_{z0}}, \quad \gamma_i = \frac{K_{zi}}{K_{z0}}, \quad \alpha_{pi} = \frac{k_{pi} H^2}{K_{z0}},$$

$$\alpha_{gi} = \frac{k_{gi} H^2}{K_{z0}}, \quad N_i = \frac{v_{di} H}{K_{zi}}, \quad N_{pi} = \frac{v_{dpi} H}{K_{zi}}, \quad (i = 1, 2)$$

$$(i) \quad Q(t) = Q_0 \delta(t)$$

$$(ii) \quad Q(t) = 1 \quad (3.50)$$

$$(iii) \quad Q(t) = 1, \quad 0 \leq t \leq t_0 \\ = 0, \quad t > t_0$$

### 3.2 METHOD OF SOLUTION

Equations (3.26) and (3.32) can be written in compact form as,

$$\mathcal{L}_1 \begin{bmatrix} C_1 \\ C_{p1} \end{bmatrix} - \begin{bmatrix} \alpha_1 + \alpha_{g1} & 0 \\ -\alpha_1 & \alpha_{p1} \end{bmatrix} \begin{bmatrix} C_1 \\ C_{p1} \end{bmatrix} = 0 \quad (3.51)$$

where  $\mathcal{L}_1$  is the advection/diffusion operator

$$\mathcal{L}_1 \equiv -\frac{\partial}{\partial t} - u_1 \frac{\partial}{\partial x} + w_1 \frac{\partial}{\partial z} + \beta_1 \frac{\partial^2}{\partial y^2} + \gamma_1 \frac{\partial^2}{\partial z^2}$$

Following the same method as in the previous chapter, we get the uncoupled system for patch I,

$$\mathcal{L}_1 C_1 - (\alpha_1 + \alpha_{g1}) C_1 = 0 \quad (3.52)$$

$$\mathcal{L}_1 B_1 - \alpha_{p1} B_1 = 0 \quad (3.53)$$

$$\text{where } B_1 = C_{p1} - \frac{\alpha_1}{\alpha_{p1} - \alpha_1 - \alpha_{g1}} C_1 \quad (3.54)$$

The conditions for  $C_1$  remains same. The corresponding conditions for  $B_1$  are,

$$B_1(x, y, z, t) = 0 \quad \text{at } t = 0 \quad (3.55)$$

$$B_1(x, y, z, t) = - \frac{\alpha_1}{\alpha_{p1} - \alpha_1 - \alpha_{g1}} \frac{Q(t)}{u_1} \delta(y) \delta(z - h_s) \quad \text{at } x = 0 \quad (3.56)$$

$$B_1(x, y, z, t) = 0 \quad \text{as } y \rightarrow \pm \infty \quad (3.57)$$

$$\frac{\partial B_1}{\partial z} = (N_{p1} - w_1) B_1 + \frac{N_{p1} - N_1}{\alpha_{p1} - \alpha_1 - \alpha_{g1}} \alpha_1 C_1 \quad \text{at } z = 0 \quad (3.58)$$

$$\frac{\partial B_1}{\partial z} = 0 \quad \text{at } z = 1 \quad (3.59)$$

Similarly we also get the uncoupled system corresponding to equations (3.38) and (3.44) for Patch-II,

$$\mathcal{L}_2 C_2 - (\alpha_2 + \alpha_{g2}) C_2 = 0 \quad (3.60)$$

$$\mathcal{L}_2 B_2 - \alpha_{p2} B_2 = 0 \quad (3.61)$$

$$\text{where } \mathcal{L}_2 \equiv - \frac{\partial}{\partial t} - u_2 \frac{\partial}{\partial x} + w_2 \frac{\partial}{\partial z} + \beta_2 \frac{\partial^2}{\partial y^2} + \gamma_2 \frac{\partial^2}{\partial z^2} \quad (3.62)$$

$$\text{and } B_2 = C_{p2} - \frac{\alpha_2}{\alpha_{p2} - \alpha_2 - \alpha_{g2}} C_2 \quad (3.63)$$

The conditions for  $C_2$  remains same. The corresponding conditions for  $B_2$  are,

$$B_2(x, y, z, t) = 0 \quad \text{at } t = 0 \quad (3.64)$$

$$B_2(x, y, z, t) = B_1(x, y, z, t) + \left[ \frac{\alpha_1}{\alpha_{p1} - \alpha_1 - \alpha_{g1}} - \frac{\alpha_2}{\alpha_{p2} - \alpha_2 - \alpha_{g2}} \right] C_1 \quad \text{at } x = x_1 \quad (3.65)$$

$$B_2(x, y, z, t) = 0 \quad \text{as } y \rightarrow \pm \infty \quad (3.66)$$

$$\frac{\partial B_2}{\partial z} = (N_{p2} - w_2)B_2 + \frac{N_{p2} - N_2}{\alpha_{p2} - \alpha_2 - \alpha_{g2}} \alpha_2 C_2 \quad \text{at } z = 0 \quad (3.67)$$

$$\frac{\partial B_2}{\partial z} = 0 \quad \text{at } z = 1 \quad (3.68)$$

Introducing the following transformations,

$$C_1(x, y, z, t) = C_{11}(x, y, z, t) \exp\left[-\frac{w_1}{2\gamma_1}(z-h_s) - \frac{w_1^2}{4\gamma_1 u_1} x\right] \quad (3.69)$$

$$B_1(x, y, z, t) = B_{11}(x, y, z, t) \exp\left[-\frac{w_1}{2\gamma_1}(z-h_s) - \frac{w_1^2}{4\gamma_1 u_1} x\right] \quad (3.70)$$

$$C_2(x, y, z, t) = C_{22}(x, y, z, t) \exp\left[-\frac{w_2}{2\gamma_2}(z-h_s) - \frac{w_2^2}{4\gamma_2 u_2} x\right] \quad (3.71)$$

$$B_2(x, y, z, t) = B_{22}(x, y, z, t) \exp\left[-\frac{w_2}{2\gamma_2}(z-h_s) - \frac{w_2^2}{4\gamma_2 u_2} x\right] \quad (3.72)$$

Equations (3.52 - 3.68) can now be written as,

Patch I ( $0 \leq x < x_1$ ,  $0 \leq z \leq 1$ )

$$\frac{\partial C_{11}}{\partial t} + u_1 \frac{\partial C_{11}}{\partial x} = \beta_1 \frac{\partial^2 C_{11}}{\partial y^2} + \gamma_1 \frac{\partial^2 C_{11}}{\partial z^2} - (\alpha_1 + \alpha_{g1}) C_{11} \quad (3.73)$$

$$C_{11}(x, y, z, t) = 0 \quad \text{at } t = 0 \quad (3.74)$$

$$C_{11}(x, y, z, t) = \frac{Q(t)}{u_1} \delta(y) \delta(z-h_s) \exp\left[-\frac{w_1}{2\gamma_1}(z-h_s)\right] \quad \text{at } x = 0 \quad (3.75)$$

$$C_{11}(x, y, z, t) = 0 \quad \text{as } y \rightarrow \pm \infty \quad (3.76)$$

$$\frac{\partial C_{11}}{\partial z} = N'_1 C_{11} \quad \text{at } z = 0 \quad (3.77)$$

$$\frac{\partial C_{11}}{\partial z} = L'_1 C_{11} \quad \text{at } z = 1 \quad (3.78)$$

$$\frac{\partial B_{11}}{\partial t} + u_1 \frac{\partial B_{11}}{\partial x} = \beta_1 \frac{\partial^2 B_{11}}{\partial y^2} + \gamma_1 \frac{\partial^2 B_{11}}{\partial z^2} - \alpha_{p1} B_{11} \quad (3.79)$$

$$B_{11}(x, y, z, t) = 0 \quad \text{at } t = 0 \quad (3.80)$$

$$B_{11}(x, y, z, t) = - \frac{\alpha_1}{\alpha_{p1} - \alpha_1 - \alpha_{g1}} \frac{Q(t)}{u_1} \delta(y) \delta(z - h_s) \exp\left(\frac{w_1}{2\gamma_1}(z - h_s)\right) \quad \text{at } x = 0 \quad (3.81)$$

$$B_{11}(x, y, z, t) = 0 \quad \text{as } y \rightarrow \pm \infty \quad (3.82)$$

$$\frac{\partial B_{11}}{\partial z} = N'_{p1} B_{11} + \frac{N_{p1} - N_1}{\alpha_{p1} - \alpha_1 - \alpha_{g1}} \alpha_1 C_{11} \quad \text{at } z = 0 \quad (3.83)$$

$$\frac{\partial B_{11}}{\partial z} = L'_1 B_{11} \quad \text{at } z = 1 \quad (3.84)$$

Patch II (  $x \geq x_1$ ,  $0 \leq z \leq 1$  )

$$\frac{\partial C_{22}}{\partial t} + u_2 \frac{\partial C_{22}}{\partial x} = \beta_2 \frac{\partial^2 C_{22}}{\partial y^2} + \gamma_2 \frac{\partial^2 C_{22}}{\partial z^2} - (\alpha_2 + \alpha_{g2}) C_{22} \quad (3.85)$$

$$C_{22}(x, y, z, t) = 0 \quad \text{at } t = 0 \quad (3.86)$$

$$C_{22}(x, y, z, t) = C_{11}(x, y, z, t) \exp\left(-\frac{1}{2}\left(\frac{w_1}{\gamma_1} - \frac{w_2}{\gamma_2}\right)(z - h_s) - \frac{1}{4}\left(\frac{w_1^2}{\gamma_1 u_1} - \frac{w_2^2}{\gamma_2 u_2}\right)x\right) \quad \text{at } x = x_1 \quad (3.87)$$

$$C_{22}(x, y, z, t) = 0 \quad \text{as } y \rightarrow \pm \infty \quad (3.88)$$

$$\frac{\partial C_{22}}{\partial z} = N_2' C_{22} \quad \text{at } z = 0 \quad (3.89)$$

$$\frac{\partial C_{22}}{\partial z} = L_2' C_{22} \quad \text{at } z = 1 \quad (3.90)$$

$$\frac{\partial B_{22}}{\partial t} + u_2 \frac{\partial B_{22}}{\partial x} = \beta_2 \frac{\partial^2 B_{22}}{\partial y^2} + \gamma_2 \frac{\partial^2 B_{22}}{\partial z^2} - \alpha_{p2} B_{22} \quad (3.91)$$

$$B_{22}(x, y, z, t) = 0 \quad \text{at } t = 0 \quad (3.92)$$

$$B_{22}(x, y, z, t) = \left[ B_{11}(x, y, z, t) + \left( \frac{\alpha_1}{\alpha_{p1} - \alpha_1 - \alpha_{g1}} - \frac{\alpha_2}{\alpha_{p2} - \alpha_2 - \alpha_{g2}} \right) C_{11} \right]$$

$$\times \exp \left( - \frac{1}{2} \left( \frac{w_1}{\gamma_1} - \frac{w_2}{\gamma_2} \right) (z - h_s) - \frac{1}{4} \left( \frac{w_1^2}{\gamma_1 u_1} - \frac{w_2^2}{\gamma_2 u_2} \right) x \right) \quad \text{at } x = x_1 \quad (3.93)$$

$$B_{22}(x, y, z, t) = 0 \quad \text{as } y \rightarrow \pm \infty \quad (3.94)$$

$$\frac{\partial B_{22}}{\partial z} = N_{p2}' B_{22} + \frac{N_{p2} - N_2}{\alpha_{p2} - \alpha_2 - \alpha_{g2}} \alpha_2 C_{22} \quad \text{at } z = 0 \quad (3.95)$$

$$\frac{\partial B_{22}}{\partial z} = L_2' B_{22} \quad \text{at } z = 1 \quad (3.96)$$

$$\text{where } N_1' = N_1 - w_1 \left( 1 - \frac{1}{2\gamma_1} \right) ; L_1' = \frac{w_1}{2\gamma_1}$$

$$N_2' = N_2 - w_2 \left( 1 - \frac{1}{2\gamma_2} \right) ; L_2' = \frac{w_2}{2\gamma_2}$$

$$N_{p1}' = N_{p1} - w_1 \left( 1 - \frac{1}{2\gamma_1} \right)$$

$$N_{p2}' = N_{p2} - w_2 \left( 1 - \frac{1}{2\gamma_2} \right)$$



### 3.3 CONCENTRATION DISTRIBUTIONS

Solutions for  $C_{11}$ ,  $B_{11}$  and  $C_{22}$ ,  $B_{22}$  are obtained using Laplace and Fourier transform techniques, (Carslaw and Jaeger, 1959) in each cases as,

#### 3.3.1 CASE I WHEN FLUX IS INSTANTANEOUS AT THE SOURCE

$$Q(t) = Q_0 \delta(t)$$

$$C_{11}(x, y, z, t) = \frac{Q_0}{u_1} P(x, y, z) \delta\left(t - \frac{x}{u_1}\right) \quad (3.97)$$

$$B_{11}(x, y, z, t) = \frac{Q_0}{u_1} Q(x, y, z) \delta\left(t - \frac{x}{u_1}\right) \quad (3.98)$$

$$C_{22}(x, y, z, t) = \frac{Q_0}{u_1} M(x, y, z) \delta\left(t - \left(\frac{x_1}{u_1} + \frac{x-x_1}{u_2}\right)\right) \quad (3.99)$$

$$B_{22}(x, y, z, t) = \frac{Q_0}{u_1} N(x, y, z) \delta\left(t - \left(\frac{x_1}{u_1} + \frac{x-x_1}{u_2}\right)\right) \quad (3.100)$$

where  $\delta(t - x)$  is the Dirac delta function defined in chapter II.

And,

$$P(x, y, z) = \frac{e^{-y^2/(4\frac{\beta_1}{u_1}x)}}{\sqrt{4\pi \frac{\beta_1}{u_1} x}} \sum_{n=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \alpha_{g1} + \gamma_1 \lambda_n^2}{u_1}\right)x\right) \frac{F_n(h_s)}{P_n} F_n(z)$$

$$Q(x, y, z) = \frac{e^{-y^2/(4\frac{\beta_1}{u_1}x)}}{\sqrt{4\pi \frac{\beta_1}{u_1} x}} \sum_{n=1}^{\infty} \frac{\alpha_1}{\alpha_{p1} - \alpha_1 - \alpha_{g1}} \exp\left(-\left(\frac{\alpha_{p1} + \gamma_1 \xi_n^2}{u_1}\right)x\right) \frac{H_n(z)}{P_{n1}}$$

$$\left( \sum_{m=1}^{\infty} (N_{p1} - N_1) \frac{\gamma_1}{u_1} \xi_n^2 \frac{F_m(h_s)}{P_m} I_{11} I_{12} - H_n(h_s) \right)$$

$$M(x, y, z) = \frac{e^{-y^2/4\beta(x)}}{\sqrt{4\pi\beta(x)}} \exp\left(-\frac{1}{4}\left(\frac{w_1^2}{\gamma_1 u_1} - \frac{w_2^2}{\gamma_2 u_2}\right)x_1\right) \sum_{n=1}^{\infty} \frac{G_n(z)}{Q_n}$$

$$\exp\left(-\left(\frac{\alpha_2 + \alpha_g \gamma_2 \mu_n^2}{u_2}\right)(x - x_1)\right) \sum_{m=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \alpha_g \gamma_1 \lambda_m^2}{u_1}\right)x_1\right) \frac{F_m(h_s)}{P_m} I_{13}$$

$$N(x, y, z) = \frac{e^{-y^2/4\beta(x)}}{\sqrt{4\pi\beta(x)}} \exp\left(-\frac{1}{4}\left(\frac{w_1^2}{\gamma_1 u_1} - \frac{w_2^2}{\gamma_2 u_2}\right)x_1\right) \sum_{n=1}^{\infty} \frac{J_n(z)}{P_{n2}}$$

$$\exp\left(-\left(\frac{\alpha_{p2} + \gamma_2 \nu_n^2}{u_2}\right)(x - x_1)\right) \left[ \sum_{r=1}^{\infty} \frac{a_{11}}{P_{r1}} \exp\left(-\left(\frac{\alpha_{p1} + \gamma_1 \xi_r^2}{u_1}\right)x_1\right) I_{14} \right]$$

$$\left\{ \sum_{m=1}^{\infty} (N_{p1} - N_1) \frac{\gamma_1}{u_1} \xi_r^2 \frac{F_m(h_s)}{P_m} I_{15} I_{16} - H_r(h_s) \right\}$$

$$+ \sum_{r=1}^{\infty} (a_{11} - a_{12}) \exp\left(-\left(\frac{\alpha_1 + \alpha_g \gamma_1 \lambda_r^2}{u_1}\right)x_1\right) \frac{F_r(h_s)}{P_r} I_{17}$$

$$+ \sum_{r=1}^{\infty} (N_{p2} - N_2) \frac{a_{12}}{Q_r} \frac{\gamma_2}{u_2} \nu_n^2 I_{18} I_{19} \sum_{m=1}^{\infty} \frac{F_m(h_s)}{P_m}$$

$$\exp\left(-\left(\frac{\alpha_1 + \alpha_g \gamma_1 \lambda_m^2}{u_1}\right)x_1\right) I_{20} \Bigg]$$

$$F_n(z) = \cos \lambda_n z + \frac{N_1'}{\lambda_n} \sin \lambda_n z$$

$$G_n(z) = \cos \mu_n z + \frac{N'_2}{\mu_n} \sin \mu_n z$$

$$H_n(z) = \cos \xi_n z + \frac{N'_{p1}}{\xi_n} \sin \xi_n z$$

$$J_n(z) = \cos \nu_n z + \frac{N'_{p2}}{\nu_n} \sin \nu_n z$$

$$P_n = \int_0^1 \left( \cos \lambda_n z + \frac{N'_1}{\lambda_n} \sin \lambda_n z \right)^2 dz$$

$$Q_n = \int_0^1 \left( \cos \mu_n z + \frac{N'_2}{\mu_n} \sin \mu_n z \right)^2 dz$$

$$P_{n1} = \int_0^1 \left( \cos \xi_n z + \frac{N'_{p1}}{\xi_n} \sin \xi_n z \right)^2 dz$$

$$P_{n2} = \int_0^1 \left( \cos \nu_n z + \frac{N'_{p2}}{\nu_n} \sin \nu_n z \right)^2 dz$$

$\lambda_n$ ,  $\mu_n$ ,  $\xi_n$  and  $\nu_n$  are the roots of the following transcendental equations respectively,

$$\tan \lambda_n = \frac{\lambda_n (N'_1 - L'_1)}{\lambda_n^2 + N'_1 L'_1}$$

$$\tan \mu_n = \frac{\mu_n (N'_2 - L'_2)}{\mu_n^2 + N'_2 L'_2}$$

$$\tan \xi_n = \frac{\xi_n (N'_{p1} - L'_1)}{\xi_n^2 + N'_{p1} L'_1}$$

$$\tan \nu_n = \frac{\nu_n (N'_{p2} - L'_2)}{\nu_n^2 + N'_{p2} L'_2}, \quad n = 1, 2, 3, \dots$$

$$I_{11} = \int_0^1 \frac{L'_1(z-1) + 1}{L'_1 - N'_{p1}(1-L'_1)} H_n(z) dz$$

$$I_{12} = \int_0^x \exp \left( - \left( \frac{\alpha_1 + \alpha_{g1} - \alpha_{p1} + \gamma_1 \lambda_m^2 - \gamma_1 \xi_n^2}{u_1} \right) x' \right) dx'$$

$$I_{13} = \int_0^1 F_m(z) G_n(z) \exp \left( - \frac{1}{2} \left( \frac{w_1}{\gamma_1} - \frac{w_2}{\gamma_2} \right) (z - h_s) \right) dz$$

$$I_{14} = \int_0^1 \exp \left( - \frac{1}{2} \left( \frac{w_1}{\gamma_1} - \frac{w_2}{\gamma_2} \right) (z - h_s) \right) H_r(z) J_n(z) dz$$

$$I_{15} = \int_0^1 \frac{L'_1(z-1) + 1}{L'_1 - N'_{p1}(1-L'_1)} H_r(z) dz$$

$$I_{16} = \int_0^{x_1} \exp \left( - \left( \frac{\alpha_1 + \alpha_{g1} - \alpha_{p1} + \gamma_1 \lambda_m^2 - \gamma_1 \xi_r^2}{u_1} \right) x' \right) dx'$$

$$I_{17} = \int_0^1 \exp \left( - \frac{1}{2} \left( \frac{w_1}{\gamma_1} - \frac{w_2}{\gamma_2} \right) (z - h_s) \right) F_r(z) J_n(z) dz$$

$$I_{18} = \int_0^1 \frac{L'_2(z-1) + 1}{L'_2 - N'_{p2}(1-L'_2)} J_n(z) dz$$

$$I_{19} = \int_0^{x-x_1} \exp \left( - \left( \frac{\alpha_2 + \alpha_{g2} - \alpha_{p2} + \gamma_2 \mu_r^2 - \gamma_2 \nu_n^2}{u_2} \right) x' \right) dx'$$

$$I_{20} = \int_0^1 \exp \left( - \frac{1}{2} \left( \frac{w_1}{\gamma_1} - \frac{w_2}{\gamma_2} \right) (z - h_s) \right) F_m(z) G_r(z) dz$$

$$a_{11} = \frac{\alpha_1}{\alpha_{p1} - \alpha_1 - \alpha_{g1}} ; a_{12} = \frac{\alpha_2}{\alpha_{p2} - \alpha_2 - \alpha_{g2}}$$

$$\beta(x) = \frac{\beta_1}{u_1} x_1 + \frac{\beta_2}{u_2} (x - x_1)$$

3.3.2 CASE II WHEN FLUX IS CONSTANT AT THE SOURCE  $Q(t) = 1$

$$C_{11}(x, y, z, t) = \frac{1}{u_1} P(x, y, z) H\left(t - \frac{x}{u_1}\right) \quad (3.101)$$

$$B_{11}(x, y, z, t) = \frac{1}{u_1} Q(x, y, z) H\left(t - \frac{x}{u_1}\right) \quad (3.102)$$

$$C_{22}(x, y, z, t) = \frac{1}{u_1} M(x, y, z) H\left(t - \left(\frac{x_1}{u_1} + \frac{x-x_1}{u_2}\right)\right) \quad (3.103)$$

$$B_{22}(x, y, z, t) = \frac{1}{u_1} N(x, y, z) H\left(t - \left(\frac{x_1}{u_1} + \frac{x-x_1}{u_2}\right)\right) \quad (3.104)$$

From equations (3.101)-(3.104) it is observed that if  $t \rightarrow \infty$  the expressions reduce to the steady state solutions.

3.3.3 CASE III WHEN FLUX IS STEP FUNCTION TYPE AT THE SOURCE

$$Q(t) = 1, \quad 0 \leq t \leq t_0$$

$$= 0, \quad t > t_0$$

$$C_{11}(x, y, z, t) = \frac{1}{u_1} P(x, y, z) \left[ H\left(t - \frac{x}{u_1}\right) - H\left(t - t_0 - \frac{x}{u_1}\right) H(t - t_0) \right] \quad (3.105)$$

$$B_{11}(x, y, z, t) = \frac{1}{u_1} Q(x, y, z) \left[ H\left(t - \frac{x}{u_1}\right) - H\left(t - t_0 - \frac{x}{u_1}\right) H(t - t_0) \right] \quad (3.106)$$

$$C_{22}(x, y, z, t) = \frac{1}{u_1} M(x, y, z) \left[ H\left(t - \left(\frac{x_1}{u_1} + \frac{x - x_1}{u_2}\right)\right) - H\left(t - t_0 - \left(\frac{x_1}{u_1} + \frac{x - x_1}{u_2}\right)\right) H(t - t_0) \right] \quad (3.107)$$

$$B_{22}(x, y, z, t) = \frac{1}{u_1} N(x, y, z) \left[ H\left(t - \left(\frac{x_1}{u_1} + \frac{x - x_1}{u_2}\right)\right) - H\left(t - t_0 - \left(\frac{x_1}{u_1} + \frac{x - x_1}{u_2}\right)\right) H(t - t_0) \right] \quad (3.108)$$

where  $H(t-x)$  is the Heaviside function defined in chapter II.

From equations (3.105)-(3.108) it is seen that as  $t_0 \rightarrow \infty$ , these equations reduce to equations (3.101)-(3.104) respectively.

The final solutions for  $C_1$ ,  $B_1$ ,  $C_2$ ,  $B_2$  can be obtained from equations (3.69)-(3.72) by putting the values of  $C_{11}$ ,  $B_{11}$ ,  $C_{22}$ ,  $B_{22}$  from the above equations in each cases. The dimensionless concentration  $C_{p1}$  and  $C_{p2}$  can then be obtained from  $C_1$ ,  $B_1$  and  $C_2$ ,  $B_2$  in each of the above cases by the following relations,

$$C_{p1}(x, y, z, t) = B_1(x, y, z, t) + \frac{\alpha_1}{\alpha_{p1} - \alpha_1 - \alpha_{g1}} C_1(x, y, z, t)$$

$$C_{p2}(x, y, z, t) = B_2(x, y, z, t) + \frac{\alpha_2}{\alpha_{p2} - \alpha_2 - \alpha_{g2}} C_2(x, y, z, t)$$

### 3.4 DISCUSSION AND RESULTS

To see the effect of various parameters the expressions for concentration distribution of both primary and secondary species in both the patches have been computed and displayed graphically

in Figures 3.1-3.12. The parameters values used in the analysis are  $\alpha_1 = \alpha_2 = 2.77$ ,  $\alpha_{g1} = \alpha_{g2} = 2.0$ ,  $\alpha_{p1} = \alpha_{p2} = 20.0$ ,  $N_1 = 4.0$ ,  $N_2 = 4.2$ ,  $N_{p1} = 0.40$ ,  $N_{p2} = 0.42$ ,  $w_1 \& w_2 = 0.0, 1.5$ ,  $w_{1\&w_2} = 1.0$ ,  $\beta_1 = \beta_2 = 10.0$ ,  $\gamma_1 = \gamma_2 = 1.0$ ,  $h_s = 0.20$ ,  $x_1 = 0.03$ ,  $y = 0.0$ ,  $Q_{w1} = 0.0$ ,  $t_0 = 0.04$ ,  $\epsilon = 0.005$ .

It is observed that the concentration of both primary and secondary pollutants decrease as downwind distance increases in all the three cases and as the rate of conversion of primary pollutant to secondary pollutant increases the concentration of primary pollutant decreases and that of secondary pollutant increases at a particular time and location.

When flux is instantaneous at the source, the concentration distributions of both the pollutants with downwind distance are shown in Figures 3.1-3.2 for different values of time  $t$  along  $z = 0.05$  (below the source height) and  $w_1 \& w_2 = 0.0, 1.5$  respectively. It is seen that the concentrations of both primary and secondary pollutants decrease as time increases. On comparing these figures it is also noted that for the points located below the source height, the concentrations of pollutants increase as the settling velocity increases. However, for the points above the source height, the concentration decreases as the settling velocity increases, (See Figure 3.8: where we have shown the vertical concentration profiles of primary pollutant for different settling velocities in the case of instantaneous flux).

When flux is constant at the source, the concentrations of both the pollutants with downwind distance are plotted in Figures 3.3 and 3.4 for different values of time  $t$  along  $z = 0.05$  and  $w_1 \& w_2 = 0.0, 1.5$  and it is seen that the concentrations of these

pollutants increase as time increases and reaches their respective steady values as  $t \rightarrow \infty$ . On comparing the figures it is again noted that for the points located below the source height, an increase in settling velocity increases the concentrations of pollutants and reverse is the case for the points above the source height.

When flux is step function type at the source, the concentrations of both the species decrease as time increases for  $t > t_0$  and behavior is similar to the case of constant flux for  $t \leq t_0$ . The increase in settling velocity increases the concentrations of both the species. (See Figures 3.5 & 3.6 ).

To see the effect of settling velocity more clearly we have also shown horizontal and vertical concentration profiles at a fixed time for constant and instantaneous sources.

In Figure 3.7 the concentration profiles of primary pollutant with downwind distance are shown for different values of settling velocities  $w_1$  and  $w_2$  at a fixed time  $t = 0.06$  at  $z = 0.0$  (the ground) and  $z = 0.5$  (above the source height) for constant flux at the source. It is quite apparent from the figure that with the increase in settling velocity, the concentration of the pollutant increases at the ground level while it decreases at  $z = 0.5$  i.e., for the points above the source height  $h_s = 0.2$ .

Similarly in Figures 3.8 and 3.9 we have shown vertical concentration profiles for different settling velocities at different distances  $x$  for instantaneous and constant flux respectively. Note the concentration increase with increase in settling velocity below the source height  $h_s = 0.2$  and



concentration decrease above the source height.

In Figure 3.10 the vertical concentration profiles of secondary pollutant are drawn for constant flux at the source and similar observations are made.

From the above analysis one important thing has been observed that as settling velocity increases, the concentration of pollutants above the source height decreases but increases below the source height. This is expected because after emission of pollutants from the source gravity comes into effect and heavier particles are likely to have higher settling velocity in comparison to not so heavier particles.

The effect of variation of ground level deposition velocity on the concentration distribution of primary pollutant with vertical height for a constant source at different distances  $x$  are shown in Figures 3.11 and 3.12. It is seen that the concentration decreases with increase in deposition velocity and this effect is more predominant below the source height. Also on comparing figures 3.11 (zero settling velocity,  $w_1 = w_2 = 0.0$ ) and 3.12 ( $w_1$  and  $w_2 = 1.0$ ) it is seen that the concentration has increased considerably below  $z = 0.2$  due to increase of settling velocity but has decreased above  $z = 0.2$ .

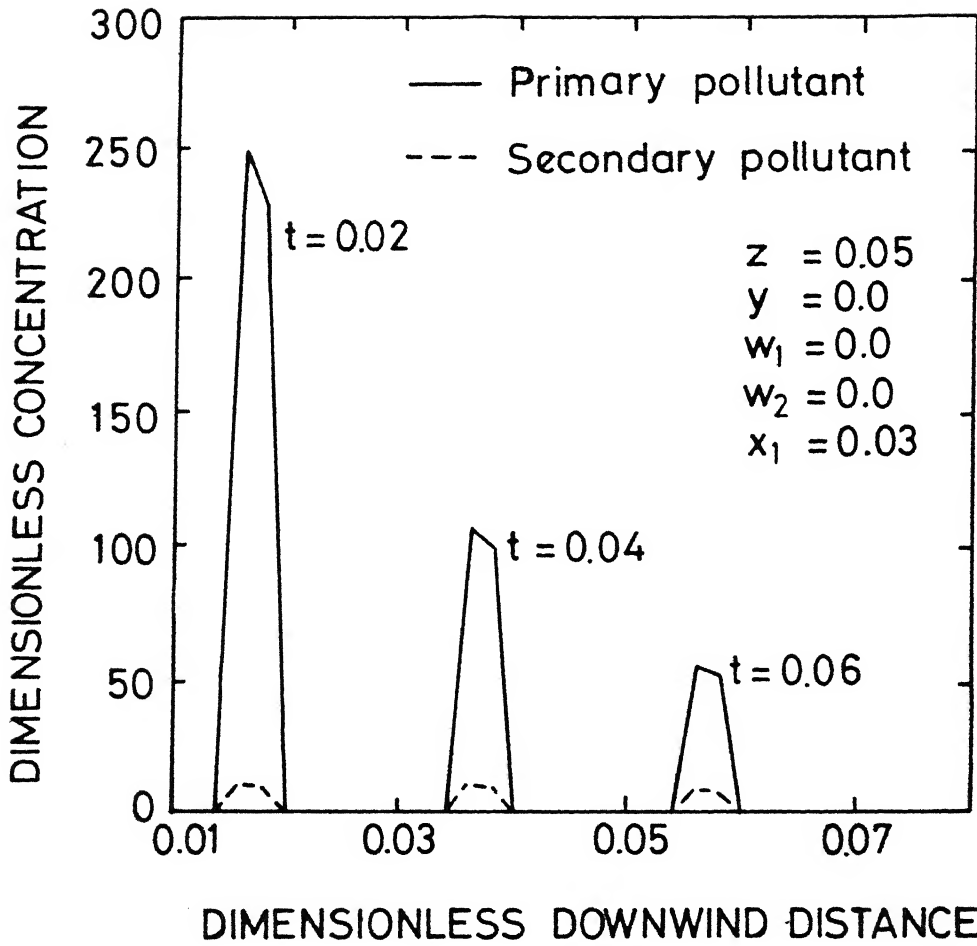


FIG. 3.1 CONCENTRATION-DISTANCE PROFILES ALONG  $z = 0.05$ , WITHOUT SETTLING ( INSTANTANEOUS FLUX ).

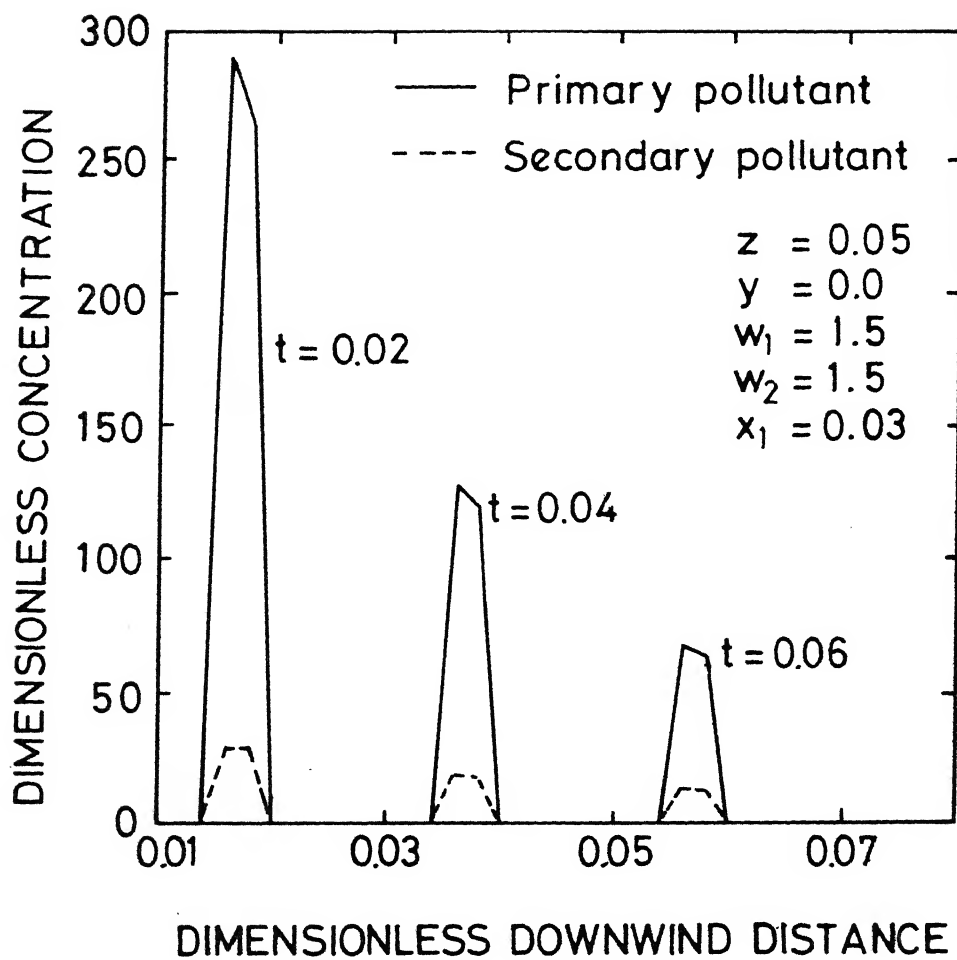


FIG.3.2 CONCENTRATION-DISTANCE PROFILES ALONG  $z=0.05$ , WITH SETTLING ( INSTANTANEOUS FLUX ).

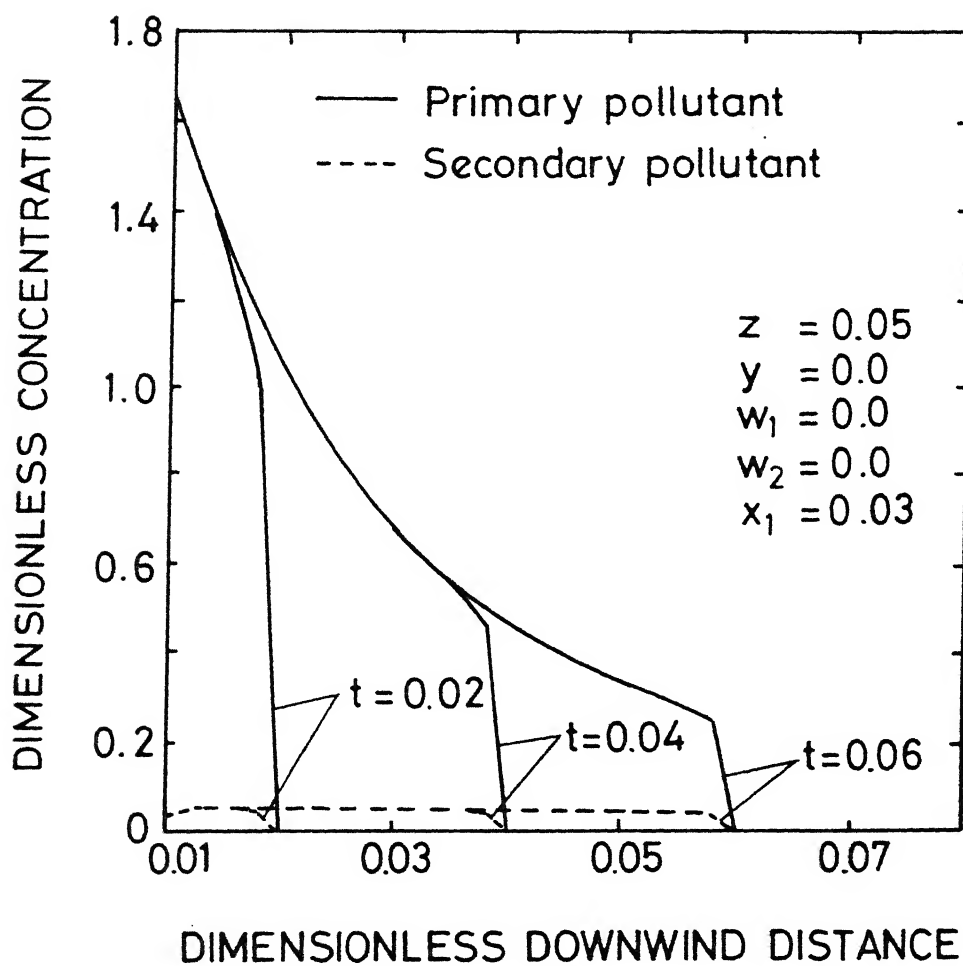


FIG.3.3 CONCENTRATION-DISTANCE PROFILES ALONG  $z = 0.05$  WITHOUT SETTLING (CONSTANT FLUX).

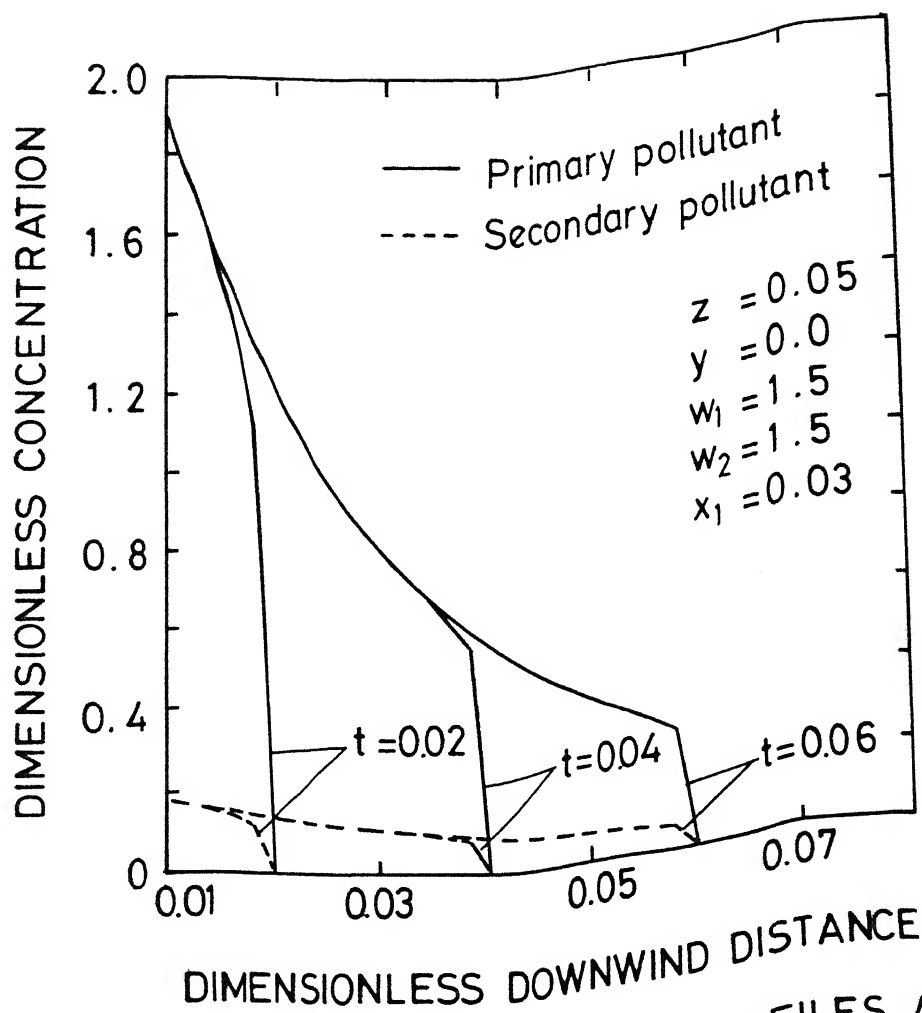


FIG. 3.4 CONCENTRATION-DISTANCE PROFILES ALONG  $z=0.05$  WITH SETTLING (CONSTANT FLUX).

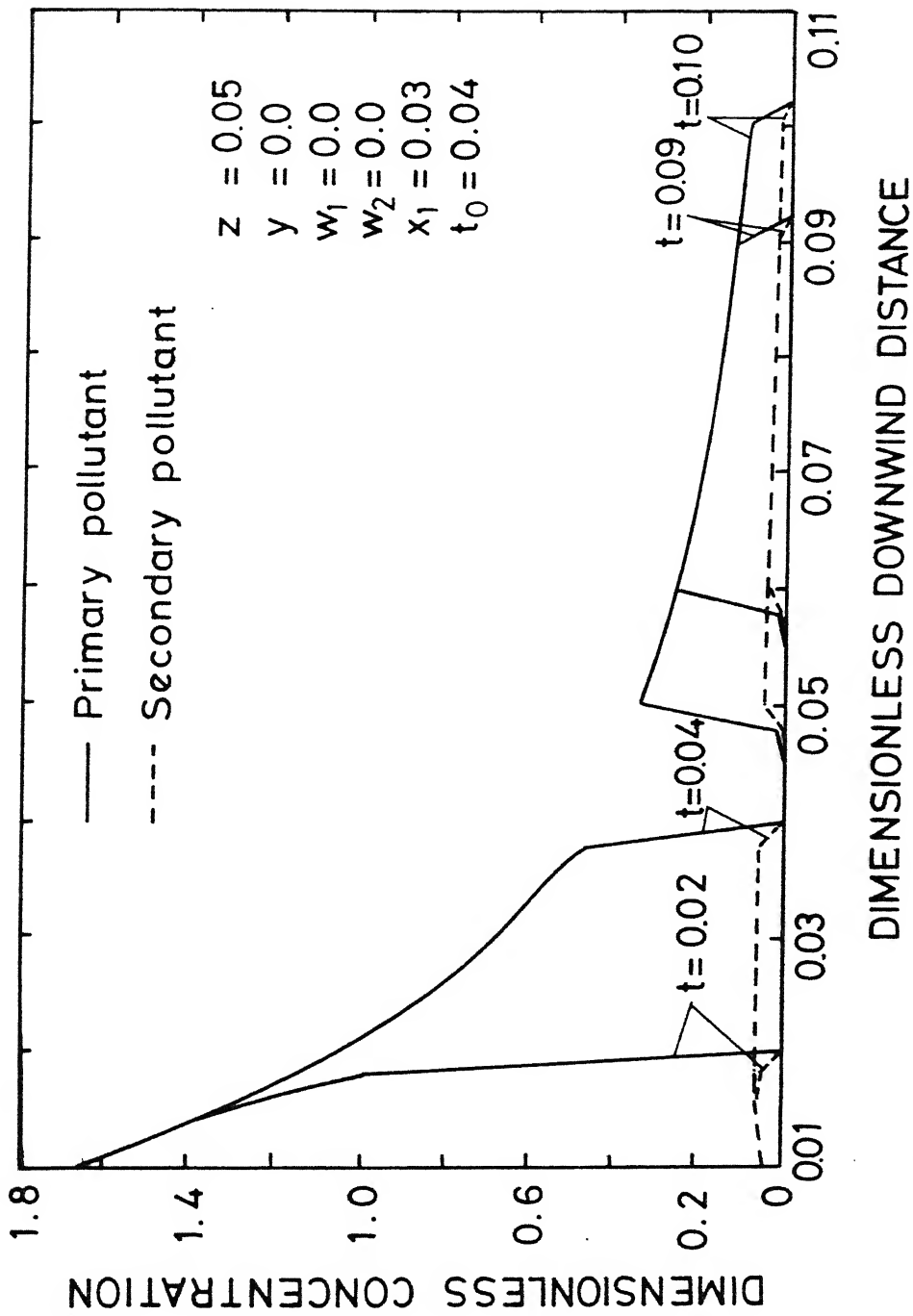


FIG.3.5 CONCENTRATION-DISTANCE PROFILES ALONG  $z = 0.05$ , WITHOUT SETTLING ( STEP FUNCTION TYPE FLUX ).

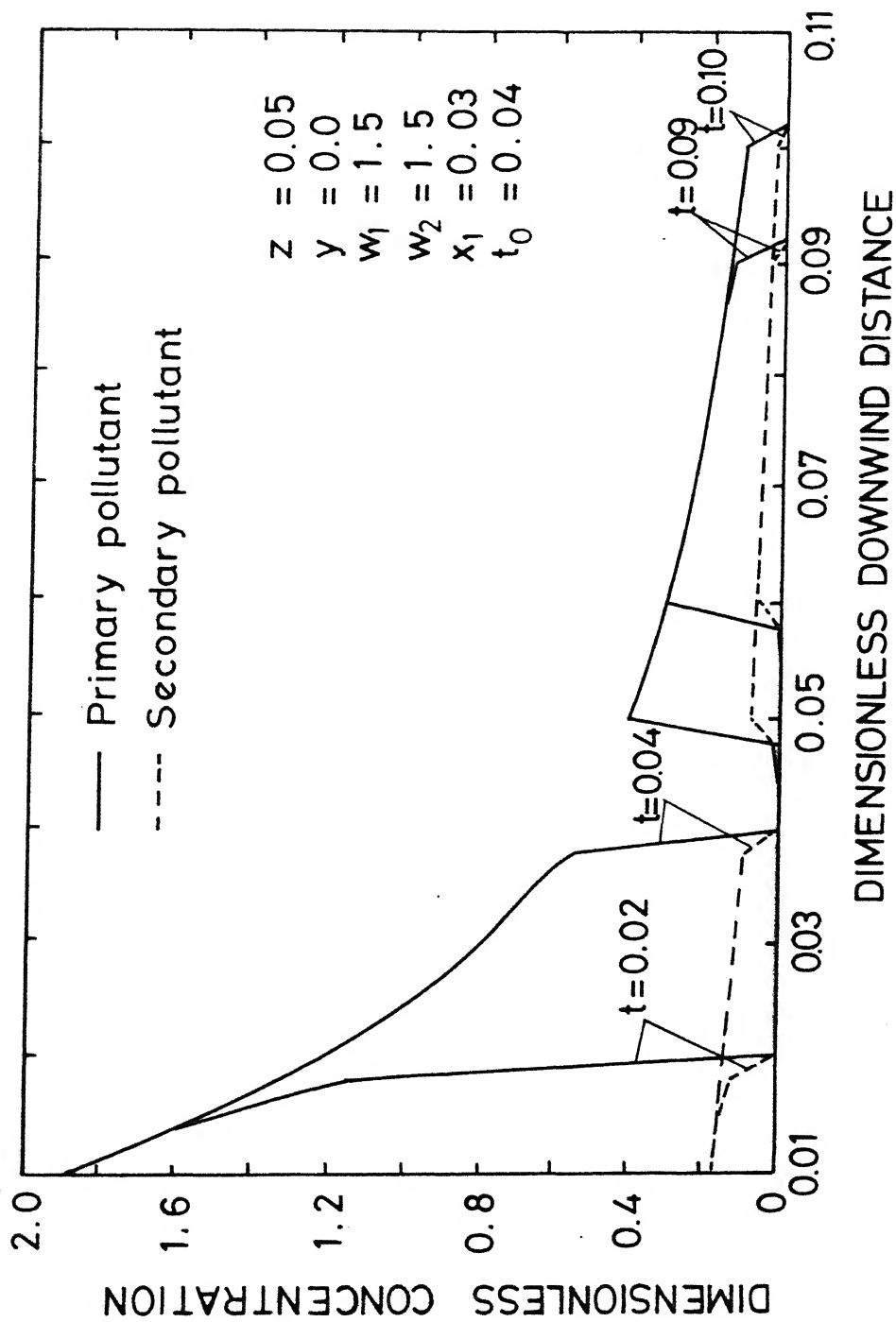


FIG. 3.6 CONCENTRATION-DISTANCE PROFILES ALONG  $z = 0.05$  WITH SETTLING ( STEP FUNCTION TYPE FLUX ).

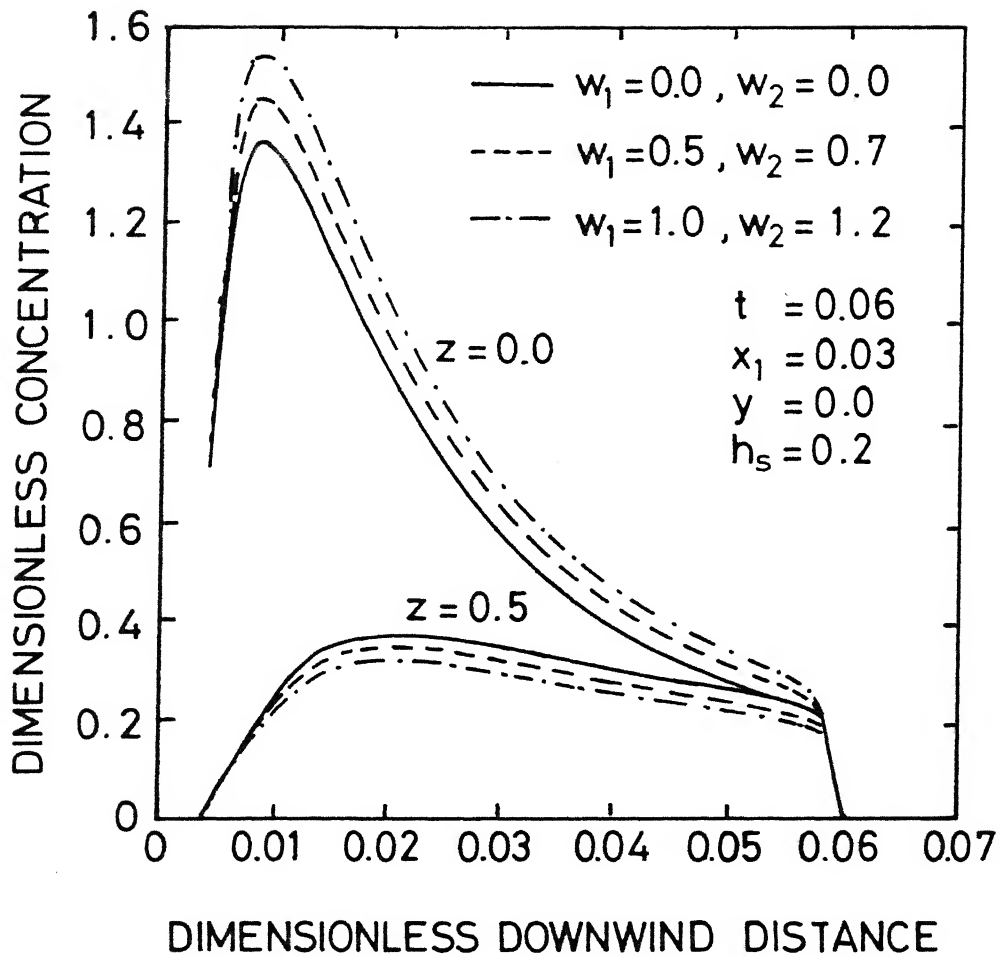
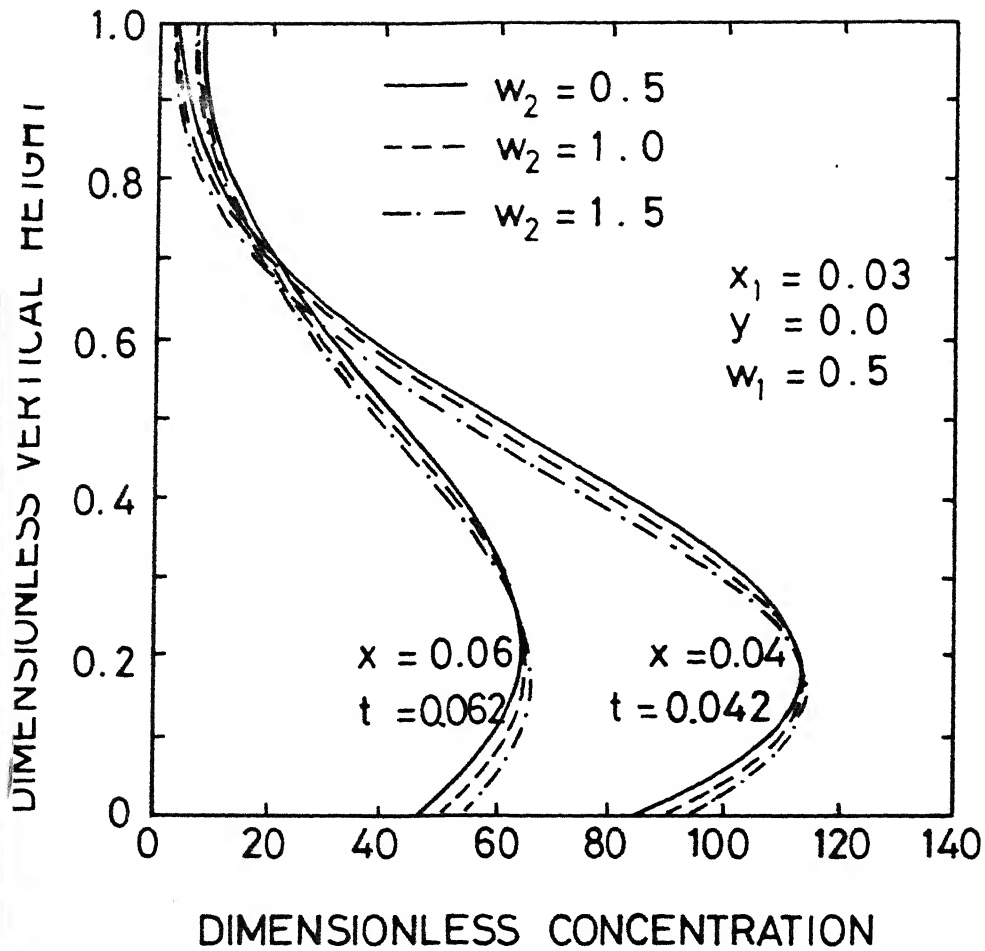


FIG.3.7 EFFECT OF SETTLING VELOCITY ON CONCENTRATION DISTRIBUTION FOR CONSTANT FLUX.





VERTICAL CONCENTRATION PROFILES FOR DIFFERENT  
SETTLING VELOCITIES (INSTANTANEOUS FLUX).

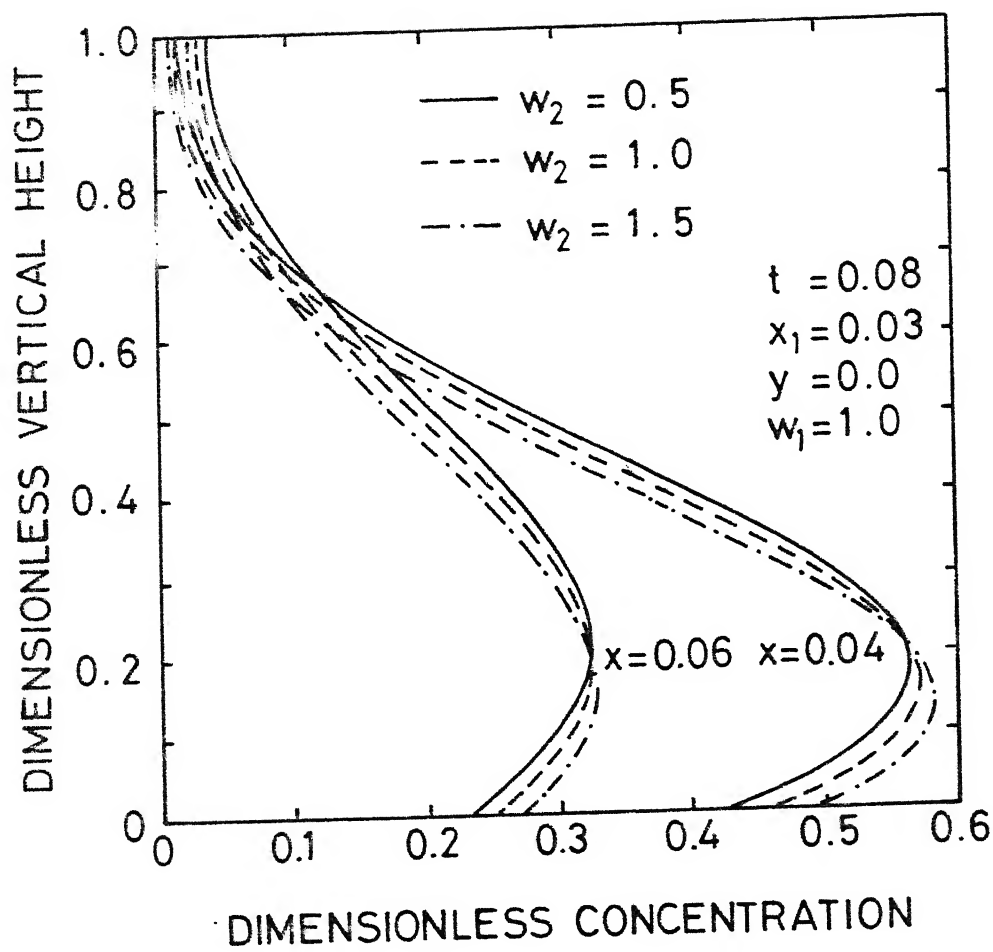


FIG.3.9 VERTICAL CONCENTRATION PROFILES FOR DIFFERENT SETTLING VELOCITIES (CONSTANT FLUX ).

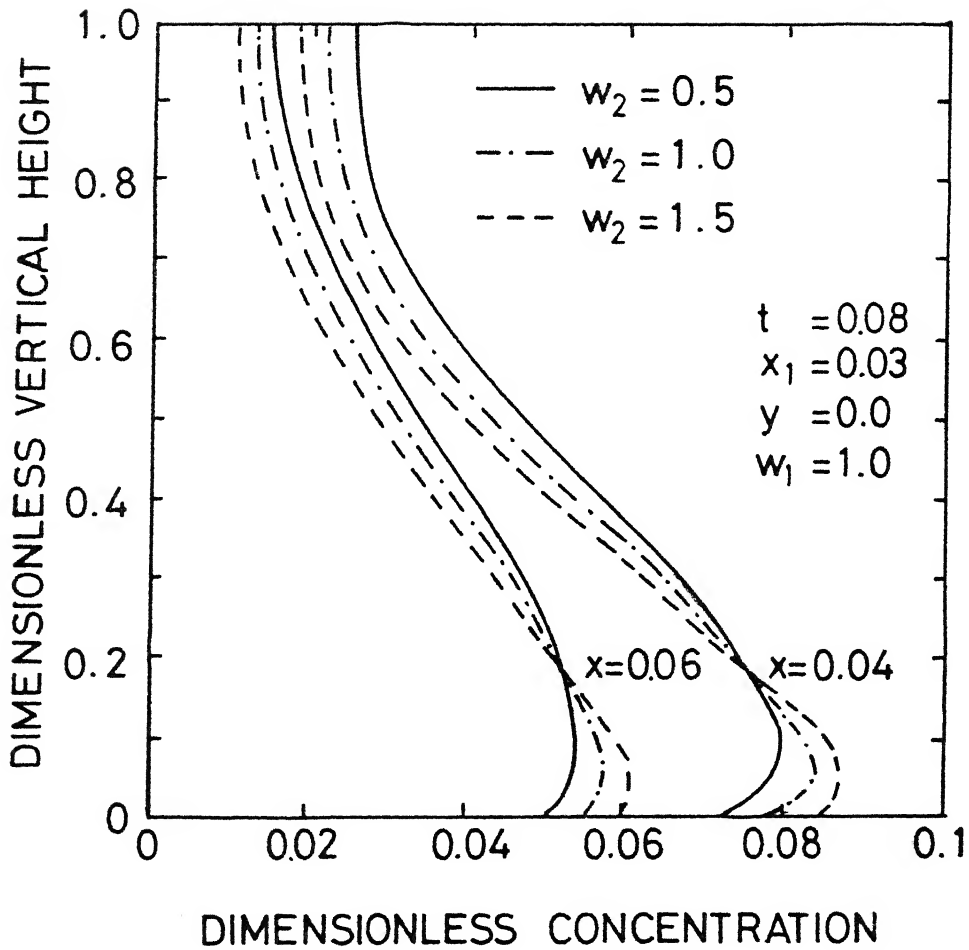


FIG.3.10 VERTICAL CONCENTRATION PROFILES OF SECONDARY POLLUTANT FOR DIFFERENT SETTLING VELOCITIES ( CONSTANT FLUX ).

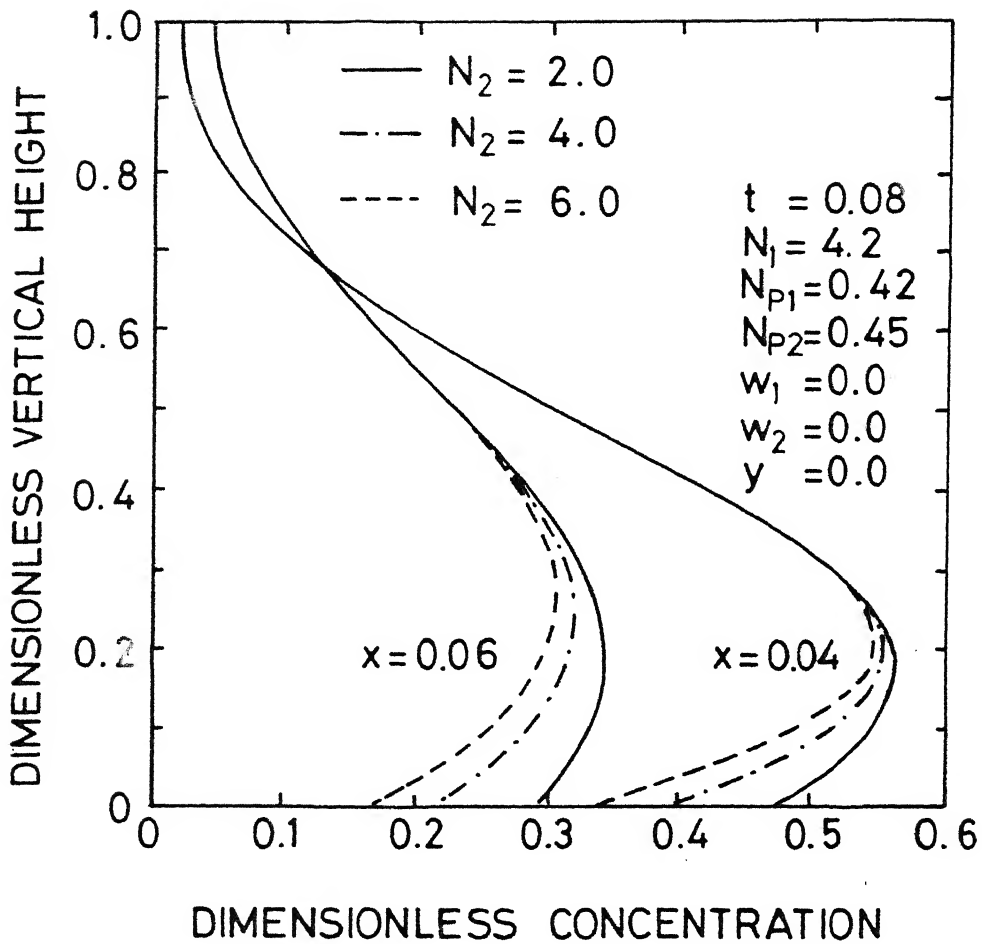


FIG.3.11 VERTICAL CONCENTRATION PROFILES FOR DIFFERENT DEPOSITION VELOCITIES, WITHOUT SETTLING (CONSTANT FLUX).

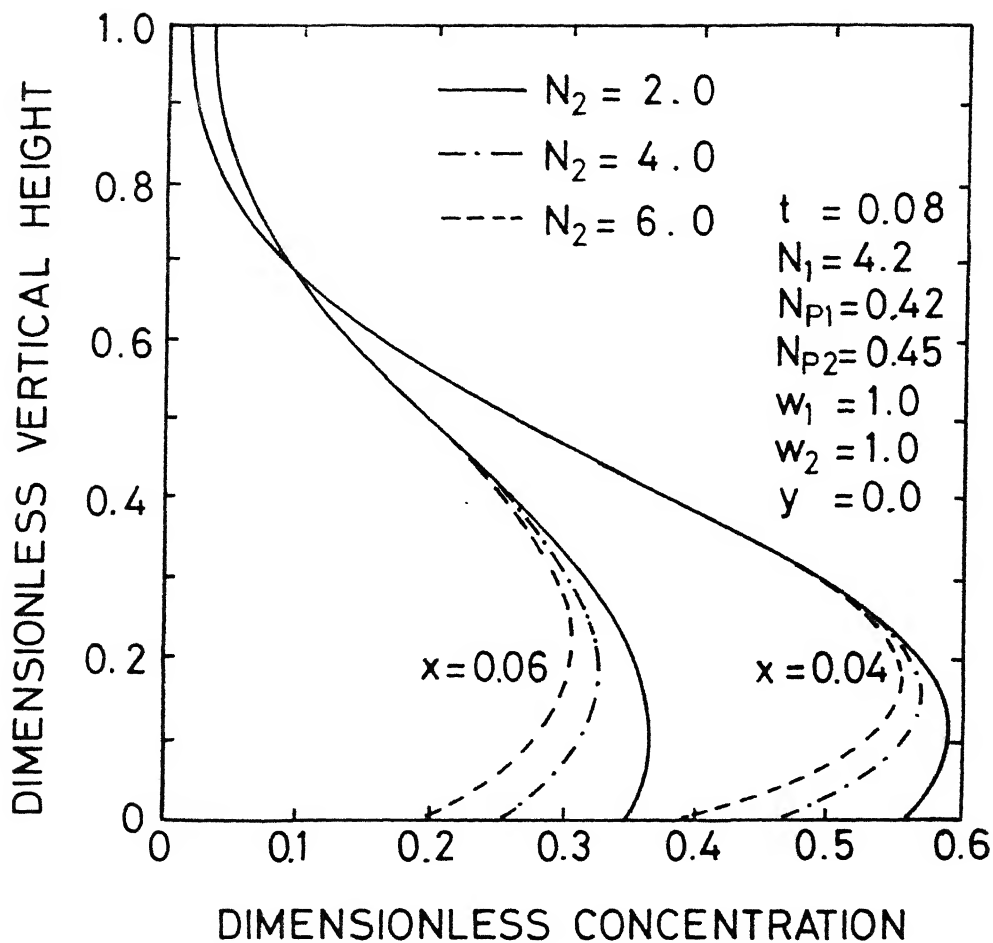


FIG.3.12 VERTICAL CONCENTRATION PROFILES FOR DIFFERENT DEPOSITION VELOCITIES; WITH SETTLING ( CONSTANT FLUX ).

## CHAPTER IV

# UNSTEADY STATE DISPERSION OF A REACTIVE AIR POLLUTANT FROM A TIME DEPENDENT POINT SOURCE : EFFECT OF GREENBELT PLANTATION

### 4.0 INTRODUCTION

The pattern of pollutant dispersion is modified by the various removal mechanisms. One such mechanism is the plantation of greenbelt, between the source and the receptor, (e.g., a habitat, a monument) capable of absorbing pollutants and inducing deposition at the surface of the canopy of trees. It is well established that certain plants have the capability of removing pollutants by absorption, deposition, etc. It may be mentioned here that these characteristics of greenbelt plantation not only depend upon the distribution, size, height and nature of the canopy but also on the type of pollutant, species of trees, shrubs, herbs, etc. planted in the greenbelt. Thus, the choice of the plantation should be such that the species planted be relatively resistant to the exposure of the specific pollutant. Number of investigations have been made in the past to study the effect of pollution on plant species, e.g. Daines(1968), Treshow(1968), Davis(1972), Takemoto and Noble(1982), Dochinger(1988), Evans(1988). In particular, survey of Indian plants in relation to atmospheric pollutants have been conducted by Ahmad *et al.*(1988) who have recommended a number of pollutant tolerant trees, shrubs and herbs for landscaping urban and industrial areas for mitigating air pollutants. The modification

of dispersion pattern of gaseous and particulate matters within plant and vegetative canopies has also been studied by many authors, e.g., MacBean(1968), Hill(1971), Bennet and Hill(1973, 1975), Chamberlain(1975a,b), O'Dell *et al.*(1977), Petit *et al.*(1976), Bache(1979a,b), Smith(1981), Hosker and Lindberg(1982), Slinn(1982a), Kapoor and Gupta(1984), Wiman and Agren(1985), Wiman and Lannefors(1985), Wiman *et al.*(1985), Baldocchi *et al.*(1987), Shukla and Chauhan(1987), Shukla *et al.*(1987). In particular, Petit *et al.*(1976) presented some results concerning characteristics of air flow within and above a forest and calculated SO<sub>2</sub> fluxes at the top of the canopy to understand the diffusion mechanism of SO<sub>2</sub>. Bache(1979) has also developed some analysis and suggested a modified form of diffusion equation to understand particulate transport mechanism within plant canopies and also compared analytical solutions with numerical results. Slinn(1982a) gave a theoretical framework to predict particle deposition to vegetative canopies and obtained approximate solutions of diffusion equation describing the air concentration of particles using variable wind velocity profile. A review of the atmospheric deposition and plant assimilation of gases and particles has been presented by Hosker and Lindberg(1982) and Smith(1981). Wiman and Agren(1985) developed a two dimensional steady state model describing aerosol concentration within forest, assumed to be very long and homogeneous in the direction perpendicular to the wind direction, by considering the interaction between forest structure, open field, forest aerodynamics and aerosol characteristics.

From these studies it may be speculated that if a greenbelt, capable of absorbing the pollutant, is planted suitably between the source and the region to be protected, it is possible to minimize the effect of pollution on this region. Flemming(1967), Bernatzky(1968), Hanson and Throne(1970), Warren(1973), Gupta and Kapoor(1985). In this direction Kapoor and Gupta(1984) have studied the effect of greenbelt on reduction of concentration of the pollutant emitted from ground level sources under steady state conditions using Gaussian plume type model.

It may be noted here that in real situations, however, pollutant sources are time dependent (such as in the case of accidental explosion of toxic gas storages), it is necessary to model the phenomenon, in general, as a dynamic process which includes the effects of stack height, location, thickness and height of the greenbelt, the location and the height of the receptor, etc.

In this chapter we, therefore, study the unsteady state dispersion of a reactive air pollutant emitted from a time dependent point source and its reduction due to greenbelt. The optimum location of the greenbelt between the source and the receptor for maximum concentration reduction of the pollutant at the receptor has also been studied. The problem is investigated by solving the unsteady state three dimensional convective diffusion equation with removal terms using suitable matching and boundary conditions.



#### 4.1 MATHEMATICAL MODEL - I : THE CASE WITH DEPOSITION AT THE TOP OF THE GREENBELT

Consider the unsteady state dispersion of a reactive air pollutant from a time dependent point source in presence of greenbelt under inversion condition. It is assumed that the greenbelt of mean thickness  $d$  and height  $h_g$  is located at a distance  $x_1$  from the source of height  $h_s$  in the wind direction extending in  $y$  direction symmetrically. The physical situation is illustrated in Figure 4.1. In modelling the process of the effect of greenbelt on pollutant distribution, we are ignoring the ecological aspects such as the internal mechanisms like distribution of leaves, locations of deposition, effect of pollutant on plants, etc. as our main concern here is to see the effect of gross depletion parameter characterizing the greenbelt which is acting as a sink, Petit *et al.*(1976), Bache(1979), Slinn(1982a). In the greenbelt region we use simplified convective diffusion equation with removal term characterizing the greenbelt in such a way that different removal parameters can be chosen for different greenbelts, Slinn(1982a), Wiman and Agren(1985). The vertical and horizontal diffusion processes in this region are also neglected due to denseness of the plant canopies, shrubs grown on the ground below canopies, etc. However, in the regions without greenbelt, usual unsteady state convective diffusion equations with reaction terms are considered with suitable matching and boundary conditions at the interfaces surrounding the greenbelt. In particular, the condition used at the top of the greenbelt (i.e., at the interface of the greenbelt region and the

region above it, the region III) implies that the deposition flux is proportional to the difference between the concentration of the same pollutant within and outside the greenbelt. Region IV is the region where receptor is located. It is also assumed that the wind is sufficiently large in the regions I, III and IV so that the downwind diffusion is negligible in comparison to advection.

Under these assumptions the dynamic equations governing the concentration distribution of the pollutant in all the regions can be written as,

Region I ( $0 \leq x < x_1$ ,  $0 \leq z \leq H$ )

The differential equation governing the concentration  $C_1(x,y,z,t)$  of the pollutant in the region I is written as,

$$\frac{\partial C_1}{\partial t} + u_1 \frac{\partial C_1}{\partial x} = K_{y1} \frac{\partial^2 C_1}{\partial y^2} + K_{z1} \frac{\partial^2 C_1}{\partial z^2} - k_1 C_1 \quad (4.1)$$

where  $x$ ,  $y$ ,  $z$  are cartesian co-ordinates,  $t$  is the time,  $x$ -axis is taken in the downwind direction and  $z$ -axis vertically upwards,  $u_1$  is the mean wind velocity,  $K_{y1}$  and  $K_{z1}$  are diffusivities in  $y$  and  $z$  directions respectively, taken as constants. The constant  $k_1$  is the reaction rate coefficient of the pollutant.

The initial and boundary conditions for equation (4.1) are,

$$C_1(x,y,z,t) = 0 \quad \text{at} \quad t = 0 \quad (4.2)$$

$$C_1(x,y,z,t) = \frac{Q(t)}{u_1} \delta(y) \delta(z-h_s) \quad \text{at} \quad x = 0 \quad (4.3)$$

$$C_1(x,y,z,t) = 0 \quad \text{as} \quad y \rightarrow \pm \infty \quad (4.4)$$

$$K_{z1} \frac{\partial C_1}{\partial z} = v_{d1} C_1 \quad \text{at} \quad z = 0 \quad (4.5)$$

$$\frac{\partial C_1}{\partial z} = 0 \quad \text{at } z = H \quad (4.6)$$

where  $v_{d1}$  is the deposition velocity of the pollutant at  $z = 0$  and  $\delta(\cdot)$  is the Dirac delta function.

Region II ( $x_1 \leq x < x_2$ ,  $0 \leq z < h_g$ )

The differential equation governing the concentration  $C_2(x, y, z, t)$  of the pollutant in the region II is written as,

$$\frac{\partial C_2}{\partial t} + u_2 \frac{\partial C_2}{\partial x} = K_{y2} \frac{\partial^2 C_2}{\partial y^2} - (k_2 + \lambda) C_2 \quad (4.7)$$

where  $u_2$  is the mean wind velocity inside the greenbelt,  $K_{y2}$  and  $K_{z2}$  are diffusivities in  $y$  and  $z$  directions respectively,  $k_2$  is the reaction rate coefficient of pollutant and  $\lambda$  is the depletion rate coefficient due to greenbelt which is acting as a sink.

The initial and boundary conditions for equation (4.7) are,

$$C_2(x, y, z, t) = 0 \quad \text{at } t = 0 \quad (4.8)$$

$$C_2(x, y, z, t) = C_1(x, y, z, t) \quad \text{at } x = x_1 \quad (4.9)$$

$$C_2(x, y, z, t) = 0 \quad \text{as } y \rightarrow \pm \infty \quad (4.10)$$

Region III ( $x_1 \leq x < x_2$ ,  $h_g \leq z \leq H$ )

The differential equation governing the concentration  $C_3(x, y, z, t)$  of the pollutant in the region III is written as,

$$\frac{\partial C_3}{\partial t} + u_3 \frac{\partial C_3}{\partial x} = K_{y3} \frac{\partial^2 C_3}{\partial y^2} + K_{z3} \frac{\partial^2 C_3}{\partial z^2} - k_3 C_3 \quad (4.11)$$

where  $u_3$  is the mean wind velocity,  $K_{y3}$  and  $K_{z3}$  are diffusivities in  $y$  and  $z$  directions respectively. The constant  $k_3$  is the reaction rate coefficient of the pollutant.

The initial and boundary conditions for equation (4.11) are,

$$C_3(x, y, z, t) = 0 \quad \text{at} \quad t = 0 \quad (4.12)$$

$$C_3(x, y, z, t) = C_1(x, y, z, t) \quad \text{at} \quad x = x_1 \quad (4.13)$$

$$C_3(x, y, z, t) = 0 \quad \text{as} \quad y \rightarrow \pm \infty \quad (4.14)$$

$$K_{z3} \frac{\partial C_3}{\partial z} = v_{d3}(C_3 - C_2) \quad \text{at} \quad z = h_g \quad (4.15)$$

$$\frac{\partial C_3}{\partial z} = 0 \quad \text{at} \quad z = H \quad (4.16)$$

where  $v_{d3}$  is the deposition velocity of the pollutant at  $z = h_g$ . Here equation(4.15) implies that due to presence of greenbelt, the deposition is taking place at the top of the greenbelt ( $z=h_g$ ) and the corresponding flux is proportional to the difference of concentration of the same pollutant within and outside the greenbelt.

Region IV ( (  $x \geq x_2$ ,  $0 \leq z \leq H$  )

The differential equation governing the concentration  $C_4(x, y, z, t)$  of the pollutant in the region IV is written as,

$$\frac{\partial C_4}{\partial t} + u_4 \frac{\partial C_4}{\partial x} = K_{y4} \frac{\partial^2 C_4}{\partial y^2} + K_{z4} \frac{\partial^2 C_4}{\partial z^2} - k_4 C_4 \quad (4.17)$$

where  $u_4$  is the mean wind velocity,  $K_{y4}$  and  $K_{z4}$  are diffusivities in  $y$  and  $z$  directions respectively. The constant  $k_4$  is the reaction rate coefficient of the pollutant.

The initial and boundary conditions for equation (4.17) are,

$$C_4(x, y, z, t) = 0 \quad \text{at} \quad t = 0 \quad (4.18)$$

$$\begin{aligned} C_4(x, y, z, t) &= C_2(x, y, z, t) \quad \text{at} \quad x = x_2 ; z < h_g \\ &= C_3(x, y, z, t) \quad \text{at} \quad x = x_2 ; z \geq h_g \end{aligned} \quad (4.19)$$

$$C_4(x, y, z, t) = 0 \quad \text{as } y \rightarrow \pm \infty \quad (4.20)$$

$$K_{z4} \frac{\partial C_4}{\partial z} = v_{d4} C_4 \quad \text{at } z = 0 \quad (4.21)$$

$$\frac{\partial C_4}{\partial z} = 0 \quad \text{at } z = H \quad (4.22)$$

where  $v_{d4}$  is the deposition velocity of the pollutant at  $z = 0$ .

As in the previous chapter the following forms of time dependent flux  $Q(t)$  are considered in the analysis:

- (i) Flux is Instantaneous,  $Q(t) = Q_0 \delta(t)$
- (ii) Flux is Constant,  $Q(t) = Q_c$  (4.23)
- (iii) Flux is Step function type

$$Q(t) = Q_c, \quad 0 \leq t \leq t_0$$

$$= 0, \quad t > t_0$$

Define the following dimensionless quantities,

$$\bar{t} = \frac{K_{z0} t}{H^2}, \quad \bar{x} = \frac{K_{z0} x}{u_0 H^2}, \quad \bar{y} = \frac{y}{H}, \quad \bar{z} = \frac{z}{H}, \quad \bar{h}_s = \frac{h_s}{H}, \quad \bar{u}_i = \frac{u_i}{u_0} \quad (i = 1, 2)$$

$$\bar{C}_i = \frac{u_0 H^2}{Q_c} C_i, \quad \bar{Q}(t) = \frac{Q(t)}{Q_c}, \quad \bar{Q}_0 = \frac{Q_0}{Q_c} \frac{K_{z0}}{H^2}, \quad \bar{\lambda} = \frac{H^2 \lambda}{K_{z0}}$$

where  $K_{z0}$  and  $u_0$  are reference diffusion coefficient and wind velocity respectively.

The equations (4.1)-(4.23) can be written in dimensionless form (dropping bars for convenience) as :

Region I  $(0 \leq x < x_1, \quad 0 \leq z \leq 1)$

$$\frac{\partial C_1}{\partial t} + u_1 \frac{\partial C_1}{\partial x} = \beta_1 \frac{\partial^2 C_1}{\partial y^2} + \gamma_1 \frac{\partial^2 C_1}{\partial z^2} - \alpha_1 C_1 \quad (4.24)$$

$$C_1(x, y, z, t) = 0 \quad \text{at } t = 0 \quad (4.25)$$

$$C_1(x, y, z, t) = \frac{Q(t)}{u_1} \delta(y) \delta(z - h_s) \quad \text{at } x = 0 \quad (4.26)$$

$$C_1(x, y, z, t) = 0 \quad \text{as } y \rightarrow \pm \infty \quad (4.27)$$

$$\frac{\partial C_1}{\partial z} = N_1 C_1 \quad \text{at } z = 0 \quad (4.28)$$

$$\frac{\partial C_1}{\partial z} = 0 \quad \text{at } z = 1 \quad (4.29)$$

Region II  $(x_1 \leq x < x_2, \quad 0 \leq z < h_g)$

$$\frac{\partial C_2}{\partial t} + u_2 \frac{\partial C_2}{\partial x} = \beta_2 \frac{\partial^2 C_2}{\partial y^2} - (\alpha_2 + \lambda) C_2 \quad (4.30)$$

$$C_2(x, y, z, t) = 0 \quad \text{at } t = 0 \quad (4.31)$$

$$C_2(x, y, z, t) = C_1(x, y, z, t) \quad \text{at } x = x_1 \quad (4.32)$$

$$C_2(x, y, z, t) = 0 \quad \text{as } y \rightarrow \pm \infty \quad (4.33)$$

Region III  $(x_1 \leq x < x_2, \quad h_g \leq z \leq 1)$

$$\frac{\partial C_3}{\partial t} + u_3 \frac{\partial C_3}{\partial x} = \beta_3 \frac{\partial^2 C_3}{\partial y^2} + \gamma_3 \frac{\partial^2 C_3}{\partial z^2} - \alpha_3 C_3 \quad (4.34)$$

$$C_3(x, y, z, t) = 0 \quad \text{at } t = 0 \quad (4.35)$$

$$C_3(x, y, z, t) = C_1(x, y, z, t) \quad \text{at } x = x_1 \quad (4.36)$$

$$C_3(x, y, z, t) = 0 \quad \text{as } y \rightarrow \pm \infty \quad (4.37)$$

$$\frac{\partial C_3}{\partial z} = N_3 (C_3 - C_2) \quad \text{at } z = h_g \quad (4.38)$$

$$\frac{\partial C_3}{\partial z} = 0 \quad \text{at } z = 1 \quad (4.39)$$

Region IV (  $x \geq x_2$  ,  $0 \leq z \leq 1$  )

$$\frac{\partial C_4}{\partial t} + u_4 \frac{\partial C_4}{\partial x} = \beta_4 \frac{\partial^2 C_4}{\partial y^2} + \gamma_4 \frac{\partial^2 C_4}{\partial z^2} - \alpha_4 C_4 \quad (4.40)$$

$$C_4(x, y, z, t) = 0 \quad \text{at} \quad t = 0 \quad (4.41)$$

$$\begin{aligned} C_4(x, y, z, t) &= C_2(x, y, z, t) \quad \text{at} \quad x = x_2 ; z < h_g \\ &= C_3(x, y, z, t) \quad \text{at} \quad x = x_2 ; z \geq h_g \end{aligned} \quad (4.42)$$

$$C_4(x, y, z, t) = 0 \quad \text{as} \quad y \rightarrow \pm \infty \quad (4.43)$$

$$\frac{\partial C_4}{\partial z} = N_4 C_4 \quad \text{at} \quad z = 0 \quad (4.44)$$

$$\frac{\partial C_4}{\partial z} = 0 \quad \text{at} \quad z = 1 \quad (4.45)$$

$$\text{where } \alpha_i = \frac{k_i H^2}{K_{z0}} , \quad \beta_i = \frac{K_{yi}}{K_{z0}} , \quad \gamma_i = \frac{K_{zi}}{K_{z0}} , \quad N_i = \frac{v_{di} H}{K_{zi}} ,$$

$$(i) \quad Q(t) = Q_0 \delta(t)$$

$$(ii) \quad Q(t) = 1 \quad (4.46)$$

$$\begin{aligned} (iii) \quad Q(t) &= 1, \quad 0 \leq t \leq t_0 \\ &= 0, \quad t > t_0 \end{aligned}$$

## 4.2 SOLUTION OF THE MODEL

The solution of equations (4.24-4.45) are obtained using

$$\frac{\beta_1}{u_1} = \frac{\beta_2}{u_2} = \frac{\beta_3}{u_3} = \frac{\beta_4}{u_4} \quad \text{in each cases as follows,}$$

### 4.2.1 CASE I WHEN FLUX IS INSTANTANEOUS AT THE SOURCE

$$Q(t) = Q_0 \delta(t)$$

$$C_1(x, y, z, t) = \frac{Q_0}{u_1} P(x, y, z) \delta\left(t - \frac{x}{u_1}\right) \quad (4.47)$$

$$C_2(x, y, z, t) = \frac{Q_0}{u_1} Q(x, y, z) \delta\left(t - \left(\frac{x_1}{u_1} + \frac{x-x_1}{u_2}\right)\right) \quad (4.48)$$

$$C_3(x, y, z, t) = \frac{Q_0}{u_1} M_1(x, y, z, t) \quad (4.49)$$

$$C_4(x, y, z, t) = \frac{Q_0}{u_1} N_1(x, y, z, t) \quad (4.50)$$

where

$$P(x, y, z) = \frac{e^{-y^2/(4\frac{\beta_1}{u_1}x)}}{\sqrt{4\pi \frac{\beta_1}{u_1} x}} \sum_{n=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \gamma_1 \lambda_n^2}{u_1}\right)x\right) \frac{F_n(h_s)}{P_n} F_n(z)$$

$$Q(x, y, z) = \frac{e^{-y^2/(4\frac{\beta_1}{u_1}x)}}{\sqrt{4\pi \frac{\beta_1}{u_1} x}} \sum_{n=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \gamma_1 \lambda_n^2}{u_1}x_1 + \frac{\alpha_2 + \lambda}{u_2}(x - x_1)\right)\right) \frac{F_n(h_s)}{P_n} F_n(z)$$

$$M_1(x, y, z, t) = \frac{e^{-y^2/(4\frac{\beta_1}{u_1}x)}}{\sqrt{4\pi \frac{\beta_1}{u_1} x}} \sum_{n=1}^{\infty} \exp\left(-\left(\frac{\alpha_3 + \gamma_3 \mu_n^2}{u_3}\right)(x - x_1)\right) \frac{G_n(z-h_g)}{Q_n}$$

$$\left[ \sum_{m=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \gamma_1 \lambda_m^2}{u_1}\right)x_1\right) \frac{F_m(h_s)}{P_m} \int_{h_g}^1 F_m(z) G_n(z-h_g) dz \right.$$

$$\delta\left(t - \left(\frac{x_1}{u_1} + \frac{x-x_1}{u_3}\right)\right) + \frac{\gamma_3}{u_3} \mu_n^2 \int_{h_g}^1 G_n(z-h_g) dz \sum_{m=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \gamma_1 \lambda_m^2}{u_1}\right)x_1\right)$$

$$\left. \frac{F_m(h_s)}{P_m} F_m(h_g) \left\{ f_{n1} - f_{n2} \exp\left(-\left(\frac{\alpha_2 + \lambda}{u_2} - \frac{\alpha_3 + \gamma_3 \mu_n^2}{u_3}\right)(x - x_1)\right)\right\} \right]$$



$$N_1(x, y, z, t) = \frac{e^{-y^2/(4\frac{\beta_1}{u_1}x)}}{\sqrt{4\pi\frac{\beta_1}{u_1}x}} \sum_{n=1}^{\infty} \exp\left(-\left(\frac{\alpha_4 + \gamma_4 \nu_n^2}{u_4}\right)(x - x_2)\right) \frac{H_n(z)}{P_{n1}}$$

$$\left[ \sum_{k=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \gamma_1 \lambda_k^2}{u_1}\right)x_1 + \frac{\alpha_2 + \lambda}{u_2}(x_2 - x_1)\right)\right] \frac{F_k(h_s)}{P_k} \int_0^{h_g} F_k(z) H_n(z) dz$$

$$\delta\left(t - \left(\frac{x_1}{u_1} + \frac{x_2 - x_1}{u_2} + \frac{x - x_2}{u_4}\right)\right) + \sum_{k=1}^{\infty} \exp\left(-\left(\frac{\alpha_3 + \gamma_3 \mu_k^2}{u_3}\right)(x_2 - x_1)\right)$$

$$\frac{1}{Q_k} \int_{h_g}^1 G_k(z - h_g) H_n(z) dz \sum_{m=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \gamma_1 \lambda_m^2}{u_1}\right)x_1\right) \frac{F_m(h_s)}{P_m}$$

$$\int_{h_g}^1 F_m(z) G_k(z - h_g) dz \delta\left(t - \left(\frac{x_1}{u_1} + \frac{x_2 - x_1}{u_3} + \frac{x - x_2}{u_4}\right)\right)$$

$$+ \sum_{k=1}^{\infty} \frac{\gamma_3}{u_3} \mu_k^2 \frac{1}{Q_k} \exp\left(-\left(\frac{\alpha_3 + \gamma_3 \mu_k^2}{u_3}\right)(x_2 - x_1)\right) \int_{h_g}^1 G_k(z - h_g) dz$$

$$\int_{h_g}^1 G_k(z - h_g) H_n(z) dz \sum_{m=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \gamma_1 \lambda_m^2}{u_1}\right)x_1\right) \frac{F_m(h_s)}{P_m} F_m(h_g)$$

$$\left\{ g_{k1} - g_{k2} \exp\left(-\left(\frac{\alpha_2 + \lambda}{u_2} - \frac{\alpha_3 + \gamma_3 \mu_k^2}{u_3}\right)(x_2 - x_1)\right) \right\}$$

$$F_n(z) = \cos \lambda_n z + \frac{N_1}{\lambda_n} \sin \lambda_n z$$

$$G_n(z) = \cos \mu_n z + \frac{N_3}{\mu_n} \sin \mu_n z$$

$$H_n(z) = \cos \nu_n z + \frac{N_4}{\nu_n} \sin \nu_n z$$

$$P_n = \int_0^1 \left( \cos \lambda_n z + \frac{N_1}{\lambda_n} \sin \lambda_n z \right)^2 dz$$

$$Q_n = \int_{h_g}^1 \left( \cos \mu_n(z-h_g) + \frac{N_3}{\mu_n} \sin \mu_n(z-h_g) \right)^2 dz$$

$$P_{n1} = \int_0^1 \left( \cos \nu_n z + \frac{N_4}{\nu_n} \sin \nu_n z \right)^2 dz$$

Here  $\lambda_n$ ,  $\mu_n$  and  $\nu_n$  are the roots of the following transcendental equations,

$$\lambda_n \tan \lambda_n = N_1$$

$$\mu_n \tan \mu_n(1-h_g) = N_3$$

$$\nu_n \tan \nu_n = N_4, \quad n = 1, 2, \dots$$

$$f_{n1} = \frac{u_3 u_2}{u_3 - u_2} \exp \left\{ -a_{1n} \left( t - \left( \frac{x_1}{u_1} + \frac{x - x_1}{u_3} \right) \right) \right\} H \left( t - \left( \frac{x_1}{u_1} + \frac{x - x_1}{u_3} \right) \right)$$

$$f_{n2} = \frac{u_3 u_2}{u_3 - u_2} \exp \left\{ -a_{1n} \left( t - \left( \frac{x_1}{u_1} + \frac{x - x_1}{u_2} \right) \right) \right\} H \left( t - \left( \frac{x_1}{u_1} + \frac{x - x_1}{u_2} \right) \right)$$

$$g_{k1} = \frac{u_3 u_2}{u_3 - u_2} \exp \left\{ -a_{1k} \left( t - \left( \frac{x_1}{u_1} + \frac{x_2 - x_1}{u_3} + \frac{x - x_2}{u_4} \right) \right) \right\} H \left( t - \left( \frac{x_1}{u_1} + \frac{x_2 - x_1}{u_3} + \frac{x - x_2}{u_4} \right) \right)$$

$$g_{k2} = \frac{u_3 u_2}{u_3 - u_2} \exp \left\{ -a_{1k} \left( t - \left( \frac{x_1}{u_1} + \frac{x_2 - x_1}{u_2} + \frac{x - x_2}{u_4} \right) \right) \right\} H \left( t - \left( \frac{x_1}{u_1} + \frac{x_2 - x_1}{u_2} + \frac{x - x_2}{u_4} \right) \right)$$

$$a_{1n} = \frac{(\alpha_2 + \lambda)u_3}{u_3 - u_2} - \frac{(\alpha_3 + \gamma_3 \mu_n^2)u_2}{u_3 - u_2}$$

4.2.2 CASE II WHEN FLUX IS CONSTANT AT THE SOURCE  $Q(t) = 1$

$$C_1(x, y, z, t) = \frac{1}{u_1} P(x, y, z) H\left(t - \frac{x}{u_1}\right) \quad (4.51)$$

$$C_2(x, y, z, t) = \frac{1}{u_1} Q(x, y, z) H\left(t - \left(\frac{x_1}{u_1} + \frac{x - x_1}{u_2}\right)\right) \quad (4.52)$$

$$C_3(x, y, z, t) = \frac{1}{u_1} M_2(x, y, z, t) \quad (4.53)$$

$$C_4(x, y, z, t) = \frac{1}{u_1} N_2(x, y, z, t) \quad (4.54)$$

where

$$M_2(x, y, z, t) = \frac{e^{-y^2/(4\frac{\beta_1}{u_1}x)}}{\sqrt{4\pi\frac{\beta_1}{u_1}x}} \sum_{n=1}^{\infty} \exp\left(-\left(\frac{\alpha_3 + \gamma_3 \mu_n^2}{u_3}\right)(x - x_1)\right) \frac{G_n(z - h_g)}{Q_n}$$

$$\left[ \sum_{m=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \gamma_1 \lambda_m^2}{u_1}\right)x_1\right) \frac{F_m(h_s)}{P_m} \int_{h_g}^1 F_m(z) G_n(z - h_g) dz \right.$$

$$\left. H\left(t - \left(\frac{x_1}{u_1} + \frac{x - x_1}{u_3}\right)\right) + \frac{\gamma_3}{u_3} \mu_n^2 \int_{h_g}^1 G_n(z - h_g) dz \sum_{m=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \gamma_1 \lambda_m^2}{u_1}\right)x_1\right) \right.$$

$$\left. \frac{F_m(h_s)}{P_m} F_m(h_g) \left\{ f_{n3} - f_{n4} \exp\left(-\left(\frac{\alpha_2 + \lambda}{u_2} - \frac{\alpha_3 + \gamma_3 \mu_n^2}{u_3}\right)(x - x_1)\right) \right\} \right]$$

$$N_2(x, y, z, t) = \frac{e^{-y^2/(4\frac{\beta_1}{u_1}x)}}{\sqrt{4\pi\frac{\beta_1}{u_1}x}} \sum_{n=1}^{\infty} \exp\left(-\left(\frac{\alpha_4 + \gamma_4 \mu_n^2}{u_4}\right)(x - x_2)\right) \frac{H_n(z)}{P_{n1}}$$

$$\left[ \sum_{k=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \gamma_1 \lambda_k^2}{u_1}x_1 + \frac{\alpha_2 + \lambda}{u_2}(x_2 - x_1)\right)\right) \frac{F_k(h_s)}{P_k} \int_0^{h_g} F_k(z) H_n(z) dz \right.$$

$$H\left(t - \left(\frac{x_1}{u_1} + \frac{x_2 - x_1}{u_2} + \frac{x - x_2}{u_4}\right)\right) + \sum_{k=1}^{\infty} \exp\left(-\left(\frac{\alpha_3 + \gamma_3 \mu_k^2}{u_3}\right)(x_2 - x_1)\right)$$

$$\frac{1}{Q_k} \int_{h_g}^1 G_k(z - h_g) H_n(z) dz \sum_{m=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \gamma_1 \lambda_m^2}{u_1}\right)x_1\right) \frac{F_m(h_s)}{P_m}$$

$$h_g \int_1^1 F_m(z) G_k(z - h_g) dz H\left(t - \left(\frac{x_1}{u_1} + \frac{x_2 - x_1}{u_3} + \frac{x - x_2}{u_4}\right)\right)$$

$$+ \sum_{k=1}^{\infty} \frac{\gamma_3}{u_3} \mu_k^2 \frac{1}{Q_k} \exp\left(-\left(\frac{\alpha_3 + \gamma_3 \mu_k^2}{u_3}\right)(x_2 - x_1)\right) h_g \int_1^1 G_k(z - h_g) dz$$

$$h_g \int_1^1 G_k(z - h_g) H_n(z) dz \sum_{m=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \gamma_1 \lambda_m^2}{u_1}\right)x_1\right) \frac{F_m(h_s)}{P_m} F_m(h_g)$$

$$\left\{ g_{k3} - g_{k4} \exp\left(-\left(\frac{\alpha_2 + \lambda}{u_2} - \frac{\alpha_3 + \gamma_3 \mu_k^2}{u_3}\right)(x_2 - x_1)\right) \right\}$$

$$f_{n3} = \frac{u_3 u_2}{u_3 - u_2} \left\{ \frac{1 - e^{-a_{1n} \left( t - \left( \frac{x_1}{u_1} + \frac{x - x_1}{u_3} \right) \right)}}{a_{1n}} \right\} \\ \times H \left( t - \left( \frac{x_1}{u_1} + \frac{x - x_1}{u_3} \right) \right)$$

$$f_{n4} = \frac{u_3 u_2}{u_3 - u_2} \left\{ \frac{1 - e^{-a_{1n} \left( t - \left( \frac{x_1}{u_1} + \frac{x - x_1}{u_2} \right) \right)}}{a_{1n}} \right\} \\ \times H \left( t - \left( \frac{x_1}{u_1} + \frac{x - x_1}{u_2} \right) \right)$$

$$g_{k3} = \frac{u_3 u_2}{u_3 - u_2} \left\{ \frac{1 - e^{-a_{1k} \left( t - \left( \frac{x_1}{u_1} + \frac{x_2 - x_1}{u_3} + \frac{x - x_2}{u_4} \right) \right)}}{a_{1k}} \right\} \\ \times H \left( t - \left( \frac{x_1}{u_1} + \frac{x_2 - x_1}{u_3} + \frac{x - x_2}{u_4} \right) \right)$$

$$g_{k4} = \frac{u_3 u_2}{u_3 - u_2} \left\{ \frac{1 - e^{-a_{1k} \left( t - \left( \frac{x_1}{u_1} + \frac{x_2 - x_1}{u_2} + \frac{x - x_2}{u_4} \right) \right)}}{a_{1k}} \right\} \\ \times H \left( t - \left( \frac{x_1}{u_1} + \frac{x_2 - x_1}{u_2} + \frac{x - x_2}{u_4} \right) \right)$$

#### 4.2.3 CASE III WHEN FLUX IS STEP FUNCTION TYPE AT THE SOURCE

$$Q(t) = 1, \quad 0 \leq t \leq t_0 \\ = 0, \quad t > t_0$$

$$C_1(x, y, z, t) = \frac{1}{u_1} P(x, y, z) \left( H \left( t - \frac{x}{u_1} \right) - H \left( t - t_0 - \frac{x}{u_1} \right) H(t - t_0) \right) \quad (4.55)$$

$$C_2(x, y, z, t) = \frac{1}{u_1} Q(x, y, z) \left( H\left(t - \left(\frac{x_1}{u_1} + \frac{x-x_1}{u_2}\right)\right) - H\left(t - t_0 - \left(\frac{x_1}{u_1} + \frac{x-x_1}{u_2}\right)\right) H(t-t_0) \right) \quad (4.56)$$

$$C_3(x, y, z, t) = \frac{1}{u_1} M_3(x, y, z, t) \quad (4.57)$$

$$C_4(x, y, z, t) = \frac{1}{u_1} N_3(x, y, z, t) \quad (4.58)$$

where

$$M_3(x, y, z, t) = \frac{e^{-y^2/(4\frac{\beta_1}{u_1}x)}}{\sqrt{4\pi \frac{\beta_1}{u_1}x}} \sum_{n=1}^{\infty} \exp\left(-\left(\frac{\alpha_3 + \gamma_3 \mu_n^2}{u_3}\right)(x - x_1)\right) \frac{G_n(z-h_g)}{Q_n}$$

$$\left[ \sum_{m=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \gamma_1 \lambda_m^2}{u_1}\right)x_1\right) \frac{F_m(h_s)}{P_m} h_g \int_{h_g}^1 F_m(z) G_n(z-h_g) dz \right.$$

$$\left. \left\{ H\left(t - \left(\frac{x_1}{u_1} + \frac{x-x_1}{u_3}\right)\right) - H\left(t - t_0 - \left(\frac{x_1}{u_1} + \frac{x-x_1}{u_3}\right)\right) H(t-t_0) \right\} \right.$$

$$+ \frac{\gamma_3}{u_3} \mu_n^2 h_g \int_{h_g}^1 G_n(z-h_g) dz \sum_{m=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \gamma_1 \lambda_m^2}{u_1}\right)x_1\right) \frac{F_m(h_s)}{P_m} F_m(h_g)$$

$$\left. \left\{ f_{n5} - f_{n6} \exp\left(-\left(\frac{\alpha_2 + \lambda}{u_2} - \frac{\alpha_3 + \gamma_3 \mu_n^2}{u_3}\right)(x - x_1)\right)\right\} \right]$$

$$N_3(x, y, z, t) = \frac{e^{-y^2/(4\frac{\beta_1}{u_1}x)}}{\sqrt{4\pi\frac{\beta_1}{u_1}x}} \sum_{n=1}^{\infty} \exp\left(-\left(\frac{\alpha_4 + \gamma_4 \nu_n^2}{u_4}\right)(x - x_2)\right) \frac{H_n(z)}{P_{n1}}$$

$$\left[ \sum_{k=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \gamma_1 \lambda_k^2}{u_1}x_1 + \frac{\alpha_2 + \lambda}{u_2}(x_2 - x_1)\right)\right) \frac{F_k(h_s)}{P_k} \int_0^{h_g} F_k(z) H_n(z) dz \right.$$

$$\left. \left\{ H\left(t - \left(\frac{x_1 + x_2 - x_1}{u_1} + \frac{x - x_2}{u_4}\right)\right) - H\left(t - t_0 - \left(\frac{x_1 + x_2 - x_1}{u_1} + \frac{x - x_2}{u_4}\right)\right) H(t - t_0) \right\} \right.$$

$$+ \sum_{k=1}^{\infty} \exp\left(-\left(\frac{\alpha_3 + \gamma_3 \mu_k^2}{u_3}\right)(x_2 - x_1)\right) \frac{1}{Q_k} \int_{h_g}^1 G_k(z - h_g) H_n(z) dz$$

$$\sum_{m=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \gamma_1 \lambda_m^2}{u_1}\right)x_1\right) \frac{F_m(h_s)}{P_m} \int_{h_g}^1 G_k(z - h_g) F_m(z) dz$$

$$\left\{ H\left(t - \left(\frac{x_1 + x_2 - x_1}{u_1} + \frac{x - x_2}{u_4}\right)\right) - H\left(t - t_0 - \left(\frac{x_1 + x_2 - x_1}{u_1} + \frac{x - x_2}{u_4}\right)\right) H(t - t_0) \right\}$$

$$+ \sum_{k=1}^{\infty} \frac{\gamma_3}{u_3} \mu_k^2 \frac{1}{Q_k} \exp\left(-\left(\frac{\alpha_3 + \gamma_3 \mu_k^2}{u_3}\right)(x_2 - x_1)\right) \int_{h_g}^1 G_k(z - h_g) dz$$

$$\int_{h_g}^1 G_k(z - h_g) H_n(z) dz \sum_{m=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \gamma_1 \lambda_m^2}{u_1}\right)x_1\right) \frac{F_m(h_s)}{P_m} F_m(h_g)$$

$$\left\{ g_{k5} - g_{k6} \exp\left(-\left(\frac{\alpha_2 + \lambda}{u_2} - \frac{\alpha_3 + \gamma_3 \mu_k^2}{u_3}\right)(x_2 - x_1)\right) \right\}$$

$$f_{n5} = \frac{u_3 u_2}{u_3 - u_2} \left[ \left\{ \frac{1 - e^{-a_{1n} \left( t - \left( \frac{x_1}{u_1} + \frac{x - x_1}{u_3} \right) \right)}}{a_{1n}} \right\} H \left( t - \left( \frac{x_1}{u_1} + \frac{x - x_1}{u_3} \right) \right) \right. \\ \left. - \left\{ \frac{1 - e^{-a_{1n} \left( t - t_0 - \left( \frac{x_1}{u_1} + \frac{x - x_1}{u_3} \right) \right)}}{a_{1n}} \right\} H \left( t - t_0 - \left( \frac{x_1}{u_1} + \frac{x - x_1}{u_3} \right) \right) \right. \\ \left. \times H(t - t_0) \right]$$

$$f_{n6} = \frac{u_3 u_2}{u_3 - u_2} \left[ \left\{ \frac{1 - e^{-a_{1n} \left( t - \left( \frac{x_1}{u_1} + \frac{x - x_1}{u_2} \right) \right)}}{a_{1n}} \right\} H \left( t - \left( \frac{x_1}{u_1} + \frac{x - x_1}{u_2} \right) \right) \right. \\ \left. - \left\{ \frac{1 - e^{-a_{1n} \left( t - t_0 - \left( \frac{x_1}{u_1} + \frac{x - x_1}{u_2} \right) \right)}}{a_{1n}} \right\} H \left( t - t_0 - \left( \frac{x_1}{u_1} + \frac{x - x_1}{u_2} \right) \right) \right. \\ \left. \times H(t - t_0) \right]$$

$$g_{k5} = \frac{u_3 u_2}{u_3 - u_2} \left[ \left\{ \frac{1 - e^{-a_{1k} \left( t - \left( \frac{x_1}{u_1} + \frac{x_2 - x_1}{u_3} + \frac{x - x_2}{u_4} \right) \right)}}{a_{1k}} \right\} \right. \\ \left. \times H \left( t - \left( \frac{x_1}{u_1} + \frac{x_2 - x_1}{u_3} + \frac{x - x_2}{u_4} \right) \right) \right. \\ \left. - \left\{ \frac{1 - e^{-a_{1k} \left( t - t_0 - \left( \frac{x_1}{u_1} + \frac{x_2 - x_1}{u_3} + \frac{x - x_2}{u_4} \right) \right)}}{a_{1k}} \right\} \right. \\ \left. \times H \left( t - t_0 - \left( \frac{x_1}{u_1} + \frac{x_2 - x_1}{u_3} + \frac{x - x_2}{u_4} \right) \right) H(t - t_0) \right]$$



$$g_{k6} = \frac{u_3 u_2}{u_3 - u_2} \left\{ \frac{1 - e^{-a_{1k} \left( t - \left( \frac{x_1}{u_1} + \frac{x_2 - x_1}{u_2} + \frac{x - x_2}{u_4} \right) \right)}}{a_{1k}} \right. \\
\times H \left( t - \left( \frac{x_1}{u_1} + \frac{x_2 - x_1}{u_2} + \frac{x - x_2}{u_4} \right) \right) \\
- \left. \frac{1 - e^{-a_{1k} \left( t - t_0 - \left( \frac{x_1}{u_1} + \frac{x_2 - x_1}{u_2} + \frac{x - x_2}{u_4} \right) \right)}}{a_{1k}} \right\} \\
\times H \left( t - t_0 - \left( \frac{x_1}{u_1} + \frac{x_2 - x_1}{u_2} + \frac{x - x_2}{u_4} \right) \right) H(t - t_0) \Bigg]$$

#### 4.2.4 DISCUSSION

To discuss the effect of various parameters on the concentration distributions of pollutant, the expressions obtained above have been computed, choosing suitable dimensionless values and displayed graphically in Figures 4.2 - 4.17. The parameters values chosen are  $Q_0 = 1.0$ ,  $u_i = 1.0$ , ( $i=1,3,4$ ),  $u_2 = 0.05$ ,  $\gamma_i = 1.0$ , ( $i=1,3,4$ ),  $\alpha_i = 2.77$ ,  $\lambda = 10.0$ ,  $N_1 = 0.5$ ,  $N_3 = 4.0$ ,  $N_4 = 0.4$ ,  $\beta_i = 10.0$ , ( $i=1,3,4$ ),  $\beta_2 = 0.5$ , location of receptor  $x = 0.1$ ,  $y = 0.0$ , width of greenbelt  $d = 0.002$ , height of the greenbelt  $h_g = 0.05$ ,  $t_0 = 0.12$ ,  $\epsilon = 0.005$ .

It may be noted here that the height of the source plays an important role in determining the optimum location of greenbelt between the source and the receptor to affect the maximum concentration reduction. We have, therefore, considered three cases viz,  $h_s > h_g$ ,  $h_s = h_g$ , and  $h_s < h_g$ .

When flux is instantaneous at the source, the concentration distributions with and without greenbelt at  $x = 0.1$  (receptor) in

region IV are plotted by changing the greenbelt location  $x_1$  towards the receptor to see the maximum concentration reduction for  $h_s = 0.2, 0.05, 0.002$ , in Figures 4.2 - 4.4 respectively at different receptor heights i.e.,  $z = 0.02$  and  $0.09$  (below and above the greenbelt height  $h_g = 0.05$ ) and at time  $t = 0.102$ .

When  $h_s > h_g$  (Figure. 4.2) it is seen that maximum concentration reduction takes place at the receptor when greenbelt is located closer to the receptor, and the concentration reduction is greater if the height of the receptor is less than that of the greenbelt.

For the case when  $h_s = h_g$  (Figure 4.3) and  $h_s < h_g$  (Figure 4.4), it is found that the greenbelt should be located near the source to affect maximum concentration reduction at the receptor.

It is, therefore, speculated that if the sources are ground based like storage tanks, it is desirable to surround this area by the greenbelt to avoid further spreading of pollutants. It is also noted from these figures that the concentration reduces considerably due to greenbelt.

When flux is constant at the source, the concentration distributions with and without greenbelt at the receptor  $x = 0.1$  are plotted in Figures 4.5 - 4.7 by changing the greenbelt location  $x_1$  towards the receptor for three cases of source heights as in the previous case and  $t = 0.12$  for different receptor heights  $z = 0.02$  and  $0.09$ . In this case also similar results are noticed as before.

When flux is step function type at the source, the concentration profiles are plotted in Figures 4.8 - 4.10. It is

noted that for  $t \leq t_0$  the behavior is same as in the case of constant flux but when  $t > t_0$  the concentration becomes zero at the receptor  $x = 0.1$ .

In Figures 4.11 - 4.13 vertical concentration profiles at the receptor location  $x = 0.1$  are shown for different locations of greenbelt for three cases of source heights as before for constant flux only. It is again found from these figures that for the maximum concentration reduction for  $h_s > h_g$ , the greenbelt should be nearer to the receptor while for  $h_s \leq h_g$ , the greenbelt should be closer to the source as pointed out earlier.

In Figure 4.14 the concentration profiles with and without greenbelt with downwind distance are shown for  $h_s = 0.2$ ,  $h_g = 0.05$ ,  $d = 0.004$ ,  $t = 0.2$  at two values of  $z = 0.02, 0.09$ . It is seen that the concentration is same with and without greenbelt before the greenbelt but in the greenbelt region  $x_1 = 0.06$ ,  $d = 0.004$ , concentration decreases significantly and then increases slightly beyond the greenbelt and there after decreases continuously for the points away from the greenbelt. It is concluded here that if the receptor is far away from the greenbelt the concentration difference between with and without greenbelt approaches zero.

In Figure 4.15 the effect of depletion coefficient  $\lambda$  due to greenbelt is shown on the concentration distribution at the receptor  $x = 0.1$  for  $h_s = 0.2$  for constant flux and it is found that the concentration decreases as  $\lambda$  increases.

In Figure 4.16 the concentration profiles at the receptor  $x = 0.1$  for constant source are shown for different deposition

velocities at the top of the greenbelt located at  $x_1 = 0.08$  for  $h_s = 0.2$ . It is seen that as the deposition velocity increases the concentration at the receptor decreases.

In Figure 4.17 the vertical concentration profiles at different receptor locations  $x = 0.06, 0.10, 0.14$  are displayed while the greenbelt is located at  $x_1 = 0.04$ . It is found that as the receptor moves away from the greenbelt, the concentration decreases at the receptor. Also the concentration difference between the cases with and without greenbelt, approaches zero if the receptor is far away from the greenbelt.

#### 4.3 MATHEMATICAL MODEL - II : THE CASE WITH INTER - EXCHANGE PROCESS IN THE ADJACENT LAYER TO THE TOP OF THE GREENBELT

In this case we again consider the atmosphere to be divided into four zones between the source and the receptor as in case 4.1. We consider here the inter-exchange process in the layer of thickness  $H_e$  adjacent to the top of the greenbelt in the region III. We assume that in this layer the decrease in the rate of concentration of the pollutant  $C_3$  i.e.  $\frac{\partial C_3}{\partial t}$  is proportional to  $\frac{v_e}{H_e}(C_3 - C_2)$  where  $v_e$  is the exchange velocity, (Reible et al., 1983). In such a case the equation governing the concentration  $C_3$  of the pollutant can be written as,

$$\frac{\partial C_3}{\partial t} + u_3 \frac{\partial C_3}{\partial x} = K_{y3} \frac{\partial^2 C_3}{\partial y^2} - k_3 C_3 - \frac{v_e}{H_e} (C_3 - C_2) \quad (4.59)$$

$$C_3(x, y, z, t) = 0 \quad \text{at} \quad t = 0 \quad (4.60)$$

$$C_3(x, y, z, t) = C_1(x, y, z, t) \quad \text{at} \quad x = x_1 \quad (4.61)$$

$$C_3(x,y,z,t) = 0 \quad \text{as } y \rightarrow \pm \infty \quad (4.62)$$

for  $x_1 \leq x \leq x_2$ , and  $h_g \leq z \leq H_e$ .

The concentration in region II may also change through inter-layer exchange characterized by an exchange velocity but we assume that there is no transfer of pollutants from the greenbelt, back to the adjacent thin layer as greenbelt is assumed to be a sink. Hence the equation governing the concentration  $C_2$  in the greenbelt region remains the same as in the case 4.1. Further the equations for  $C_1$  and  $C_4$  also remain same as in the case 4.1.

The equations (4.59)-(4.62) can be written in dimensionless form as, (dropping bars for convenience)

$$\frac{\partial C_3}{\partial t} + u_3 \frac{\partial C_3}{\partial x} = \beta_3 \frac{\partial^2 C_3}{\partial y^2} - \alpha_3 C_3 - v_e (C_3 - C_2) \quad (4.63)$$

$$C_3(x,y,z,t) = 0 \quad \text{at } t = 0 \quad (4.64)$$

$$C_3(x,y,z,t) = C_1(x,y,z,t) \quad \text{at } x = x_1 \quad (4.65)$$

$$C_3(x,y,z,t) = 0 \quad \text{as } y \rightarrow \pm \infty \quad (4.66)$$

$$\text{where } \bar{v}_e = \frac{v_e H^2}{K_{z0} H_e}$$

On solving the equations (4.24 - 4.33, 4.63-4.66 and 4.40 - 4.45), the solutions for  $C_3$  and  $C_4$  are given as follows whereas the solutions of  $C_1$  and  $C_2$  are same as given above in section 4.1.

#### 4.3.1 CASE I WHEN FLUX IS INSTANTANEOUS AT THE SOURCE

$$Q(t) = Q_0 \delta(t)$$

$$C_3(x,y,z,t) = \frac{Q_0}{u_1} M_1^*(x,y,z,t) \quad (4.67)$$

$$f_{11} = \frac{u_3 u_2}{u_2 - u_3} \exp \left\{ -a_{11} \left( t - \left( \frac{x_1}{u_1} + \frac{x - x_1}{u_2} \right) \right) \right\} H \left( t - \left( \frac{x_1}{u_1} + \frac{x - x_1}{u_2} \right) \right)$$

$$f_{12} = \left[ \delta \left( t - \left( \frac{x_1}{u_1} + \frac{x - x_1}{u_3} \right) \right) - \frac{v_e u_2}{u_2 - u_3} \exp \left\{ -a_{11} \left( t - \left( \frac{x_1}{u_1} + \frac{x - x_1}{u_3} \right) \right) \right\} \right. \\ \left. \times H \left( t - \left( \frac{x_1}{u_1} + \frac{x - x_1}{u_3} \right) \right) \right]$$

$$g_{11} = \frac{u_3 u_2}{u_2 - u_3} \exp \left\{ -a_{11} \left( t - \left( \frac{x_1}{u_1} + \frac{x_2 - x_1}{u_2} + \frac{x - x_2}{u_4} \right) \right) \right\} \\ \times H \left( t - \left( \frac{x_1}{u_1} + \frac{x_2 - x_1}{u_2} + \frac{x - x_2}{u_4} \right) \right)$$

$$g_{12} = \left[ \delta \left( t - \left( \frac{x_1}{u_1} + \frac{x_2 - x_1}{u_3} + \frac{x - x_2}{u_4} \right) \right) - \frac{v_e u_2}{u_2 - u_3} \right. \\ \left. \exp \left\{ -a_{11} \left( t - \left( \frac{x_1}{u_1} + \frac{x_2 - x_1}{u_3} + \frac{x - x_2}{u_4} \right) \right) \right\} H \left( t - \left( \frac{x_1}{u_1} + \frac{x_2 - x_1}{u_3} + \frac{x - x_2}{u_4} \right) \right) \right]$$

$$a_{11} = \frac{(\alpha_3 + v_e) u_2}{u_2 - u_3} - \frac{(\alpha_2 + \lambda) u_3}{u_2 - u_3}$$

4.3.2 CASE II WHEN FLUX IS CONSTANT AT THE SOURCE  $Q(t) = 1$

$$C_3(x, y, z, t) = \frac{1}{u_1} M_2^*(x, y, z, t)$$

(4.69)

$$C_4(x, y, z, t) = \frac{1}{u_1} N_2^*(x, y, z, t)$$

(4.70)

where

$$\begin{aligned}
 M_2^*(x, y, z, t) &= \frac{e^{-y^2/(4\frac{\beta_1}{u_1}x)}}{\sqrt{4\pi \frac{\beta_1}{u_1} x}} \sum_{n=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \gamma_1 \lambda_n^2}{u_1}\right)x_1\right) \\
 &\quad \left[ \frac{v_e}{u_3} f_{13} \exp\left(-\left(\frac{\alpha_2 + \lambda}{u_2}\right)(x-x_1)\right) \right. \\
 &\quad \left. + f_{14} \exp\left(-\left(\frac{\alpha_3 + v_e}{u_3}\right)(x-x_1)\right) \right] \frac{F_n(h_s)}{P_n} F_n(z) \\
 N_2^*(x, y, z, t) &= \frac{e^{-y^2/(4\frac{\beta_1}{u_1}x)}}{\sqrt{4\pi \frac{\beta_1}{u_1} x}} \sum_{n=1}^{\infty} \exp\left(-\left(\frac{\alpha_4 + \gamma_4 \lambda_n^2}{u_4}\right)(x-x_2)\right) \frac{H_n(z)}{P_{n1}} \\
 &\quad \left[ \sum_{m=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \gamma_1 \lambda_m^2}{u_1} x_1 + \frac{\alpha_2 + \lambda}{u_2} (x_2 - x_1)\right)\right) \frac{F_m(h_s)}{P_m} \left\{ \int_0^{h_g} F_m(z) H_n(z) dz \right. \right. \\
 &\quad \left. \left. H\left(t - \left(\frac{x_1}{u_1} + \frac{x_2 - x_1}{u_2} + \frac{x - x_2}{u_4}\right)\right) + \frac{v_e}{u_3} g_{13} \int_{h_g}^1 F_m(z) H_n(z) dz \right\} \right. \\
 &\quad \left. + \sum_{m=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \gamma_1 \lambda_m^2}{u_1} x_1 + \frac{\alpha_3 + v_e}{u_3} (x_2 - x_1)\right)\right) \frac{F_m(h_s)}{P_m} g_{14} \right. \\
 &\quad \left. \left. \int_{h_g}^1 F_m(z) H_n(z) dz \right] \right. \\
 f_{13} &= \frac{u_3 u_2}{u_2 - u_3} \left\{ \frac{1 - e^{-a_{11} \left(t - \left(\frac{x_1}{u_1} + \frac{x - x_1}{u_2}\right)\right)}}{a_{11}} \right\} \\
 &\quad \times H\left(t - \left(\frac{x_1}{u_1} + \frac{x - x_1}{u_2}\right)\right)
 \end{aligned}$$

$$f_{14} = \left[ 1 - \frac{v e^{u_2}}{u_2 - u_3} \left\{ \frac{1 - e^{-a_{11} \left( t - \left( \frac{x_1}{u_1} + \frac{x - x_1}{u_3} \right) \right)}}{a_{11}} \right\} \right. \\ \left. \times H \left( t - \left( \frac{x_1}{u_1} + \frac{x - x_1}{u_3} \right) \right) \right]$$

$$g_{13} = \frac{u_3 u_2}{u_2 - u_3} \left\{ \frac{1 - e^{-a_{11} \left( t - \left( \frac{x_1}{u_1} + \frac{x_2 - x_1}{u_2} + \frac{x - x_2}{u_4} \right) \right)}}{a_{11}} \right\} \\ \times H \left( t - \left( \frac{x_1}{u_1} + \frac{x_2 - x_1}{u_2} + \frac{x - x_2}{u_4} \right) \right)$$

$$g_{14} = \left[ 1 - \frac{v e^{u_2}}{u_2 - u_3} \left\{ \frac{1 - e^{-a_{11} \left( t - \left( \frac{x_1}{u_1} + \frac{x_2 - x_1}{u_3} + \frac{x - x_2}{u_4} \right) \right)}}{a_{11}} \right\} \right] \\ \times H \left( t - \left( \frac{x_1}{u_1} + \frac{x_2 - x_1}{u_3} + \frac{x - x_2}{u_4} \right) \right)$$

4.3.3 CASE III WHEN FLUX IS STEP FUNCTION TYPE AT THE SOURCE

$$Q(t) = 1, \quad 0 \leq t \leq t_0 \\ = 0, \quad t > t_0$$

(4.71)

$$C_3(x, y, z, t) = \frac{1}{u_1} M_3^*(x, y, z, t)$$

(4.72)

$$C_4(x, y, z, t) = \frac{1}{u_1} N_3^*(x, y, z, t)$$

where



$$M_3^*(x, y, z, t) = \frac{e^{-y^2/(4\frac{\beta_1}{u_1}x)}}{\sqrt{4\pi \frac{\beta_1}{u_1} x}} \sum_{n=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \gamma_1 \lambda_n^2}{u_1}\right)x_1\right)$$

$$\left[ \frac{v}{u_3} f_{15} \exp\left(-\left(\frac{\alpha_2 + \lambda}{u}\right)(x-x_1)\right) + f_{16} \exp\left(-\left(\frac{\alpha_3 + v}{u_3}\right)(x-x_1)\right) \right] \frac{F_n(h_s)}{P_n} F_n(z)$$

$$N_3^*(x, y, z, t) = \frac{e^{-y^2/(4\frac{\beta_1}{u_1}x)}}{\sqrt{4\pi \frac{\beta_1}{u_1} x}} \sum_{n=1}^{\infty} \exp\left(-\left(\frac{\alpha_4 + \gamma_4 \lambda_n^2}{u_4}\right)(x-x_2)\right) \frac{H_n(z)}{P_{n1}}$$

$$\left[ \sum_{m=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \gamma_1 \lambda_m^2}{u_1}\right)x_1 + \frac{\alpha_2 + \lambda}{u_2}(x_2 - x_1)\right) \frac{F_m(h_s)}{P_m} \left\{ \int_0^{h_g} F_m(z) H_n(z) dz \right. \right. \\ \left. \left. \left( H\left(t - \left(\frac{x_1}{u_1} + \frac{x_2 - x_1}{u_2} + \frac{x - x_2}{u_4}\right)\right) - H\left(t - t_0 - \left(\frac{x_1}{u_1} + \frac{x_2 - x_1}{u_2} + \frac{x - x_2}{u_4}\right)\right) \right) \right. \right. \\ \left. \left. H(t - t_0) \right\} + \frac{v}{u_3} g_{15} \int_{h_g}^1 F_m(z) H_n(z) dz \right]$$

$$+ \sum_{m=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \gamma_1 \lambda_m^2}{u_1}\right)x_1 + \frac{\alpha_3 + v}{u_3}(x_2 - x_1)\right) \frac{F_m(h_s)}{P_m} g_{16} \int_{h_g}^1 F_m(z) H_n(z) dz$$

$$f_{15} = f_{13} - \frac{u_3 u_2}{u_2 - u_3} \left\{ \frac{1 - e^{-a_{11} \left(t - t_0 - \left(\frac{x_1}{u_1} + \frac{x - x_1}{u_2}\right)\right)}}{a_{11}} \right. \\ \left. - H\left(t - t_0 - \left(\frac{x_1}{u_1} + \frac{x - x_1}{u_2}\right)\right) H(t - t_0) \right\}$$

$$\begin{aligned}
 f_{16} = & \left[ H\left(t - \left(\frac{x_1}{u_1} + \frac{x - x_1}{u_3}\right)\right) - H\left(t - t_0 - \left(\frac{x_1}{u_1} + \frac{x - x_1}{u_3}\right)\right) H(t - t_0) \right] \\
 & - \frac{v e^{u_2}}{u_2 - u_3} \left[ \left\{ \frac{1 - e^{-a_{11} \left(t - \left(\frac{x_1}{u_1} + \frac{x - x_1}{u_3}\right)\right)}}{a_{11}} \right\} H\left(t - \left(\frac{x_1}{u_1} + \frac{x - x_1}{u_3}\right)\right) \right. \\
 & - \left. \left\{ \frac{1 - e^{-a_{11} \left(t - t_0 - \left(\frac{x_1}{u_1} + \frac{x - x_1}{u_3}\right)\right)}}{a_{11}} \right\} H\left(t - t_0 - \left(\frac{x_1}{u_1} + \frac{x - x_1}{u_3}\right)\right) \right. \\
 & \left. \left. \times H(t - t_0) \right] \right]
 \end{aligned}$$

$$\begin{aligned}
 g_{15} = g_{13} - \frac{u_3 u_2}{u_2 - u_3} & \left\{ \frac{1 - e^{-a_{11} \left(t - t_0 - \left(\frac{x_1}{u_1} + \frac{x_2 - x_1}{u_2} + \frac{x - x_2}{u_4}\right)\right)}}{a_{11}} \right\} \\
 & H\left(t - t_0 - \left(\frac{x_1}{u_1} + \frac{x_2 - x_1}{u_2} + \frac{x - x_2}{u_4}\right)\right) H(t - t_0)
 \end{aligned}$$

$$\begin{aligned}
 g_{16} = & \left[ H\left(t - \left(\frac{x_1}{u_1} + \frac{x_2 - x_1}{u_3} + \frac{x - x_2}{u_4}\right)\right) \right. \\
 & - \left. H\left(t - t_0 - \left(\frac{x_1}{u_1} + \frac{x_2 - x_1}{u_3} + \frac{x - x_2}{u_4}\right)\right) H(t - t_0) \right] \\
 & - \frac{v e^{u_2}}{u_2 - u_3} \left[ \left\{ \frac{1 - e^{-a_{11} \left(t - \left(\frac{x_1}{u_1} + \frac{x_2 - x_1}{u_3} + \frac{x - x_2}{u_4}\right)\right)}}{a_{11}} \right\} \right. \\
 & H\left(t - \left(\frac{x_1}{u_1} + \frac{x_2 - x_1}{u_3} + \frac{x - x_2}{u_4}\right)\right) \\
 & - \left. \left\{ \frac{1 - e^{-a_{11} \left(t - t_0 - \left(\frac{x_1}{u_1} + \frac{x_2 - x_1}{u_3} + \frac{x - x_2}{u_4}\right)\right)}}{a_{11}} \right\} \right. \\
 & \left. H\left(t - t_0 - \left(\frac{x_1}{u_1} + \frac{x_2 - x_1}{u_3} + \frac{x - x_2}{u_4}\right)\right) H(t - t_0) \right]
 \end{aligned}$$

#### 4.3.4 DISCUSSION

The expressions obtained above in this case have been computed with the same set of parameter values as used for the case of 4.1. It is found that in all the corresponding figures (not all figures shown) as to the previous section, the concentration behavior is similar (No significant difference in concentration has been noted). In particular, in Figures (4.18) - (4.20) the concentration distribution of the pollutant at the receptor  $x = 0.1$  and  $z = 0.02$  for optimization of greenbelt location and the effect of inter-layer exchange velocity  $v_e$  for the instantaneous flux at the source for three heights of the source i.e.,  $h_s > h_g$ ,  $h_s = h_g$  and  $h_s < h_g$  are shown. In this case also similar results have been found for the optimization of the greenbelt location as in Figures (4.2) - (4.4). As the inter-layer exchange velocity  $v_e$  increases the concentration of the pollutant decreases at the receptor that means more pollutants from the region III are trapped in the greenbelt and since the transfer of the pollutants, from the region II, back to region III is neglected, the concentration reduces considerably.

The concentration behavior for the case of constant and step function type flux is similar and hence not shown here. The effects of other removal parameters are also same as in the previous section.

#### 4.4 MAIN RESULTS

In this chapter the effect of greenbelt on the reduction of concentration of pollutant has been studied when greenbelt is located between the source of the pollutant and the receptor. The

following results are obtained by analyzing the model,

(1) The longitudinal concentration of the pollutant along the wind direction always decreases in presence of greenbelt and this decrease is further enhanced as the magnitude of depletion coefficient parameter due to greenbelt and its size (height and width) increase.

(2) Similarly vertical concentration at a given location, after the greenbelt, decreases as the value of aforesaid parameters increase.

(3) It has been shown by using numerical optimization that the reduction in pollutant concentration at the receptor is maximum under the following conditions.

(i) When the source height is greater than the greenbelt height, the greenbelt should be located as close as possible to the receptor.

(ii) When the source height is less than or equal to the greenbelt height, the greenbelt should be located as close as possible to the source.

(4) It has also been noted in both the above cases that for maximum concentration reduction at the receptor, the height of the receptor should be as small as possible than the greenbelt height.

(5) The reduction in concentration at the receptor is larger when the deposition velocity at the top of the greenbelt or the inter-layer exchange velocity in the layer adjacent to the top of the greenbelt increases.

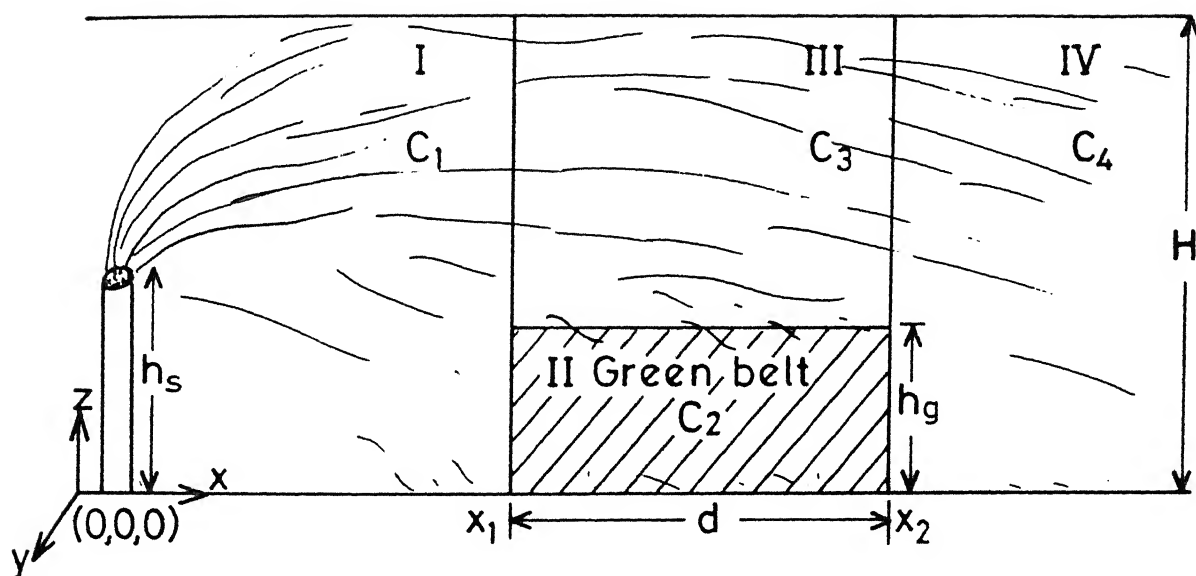


FIG. 4.1 DISPERSION OF AIR POLLUTANT IN PRESENCE OF GREENBELT.

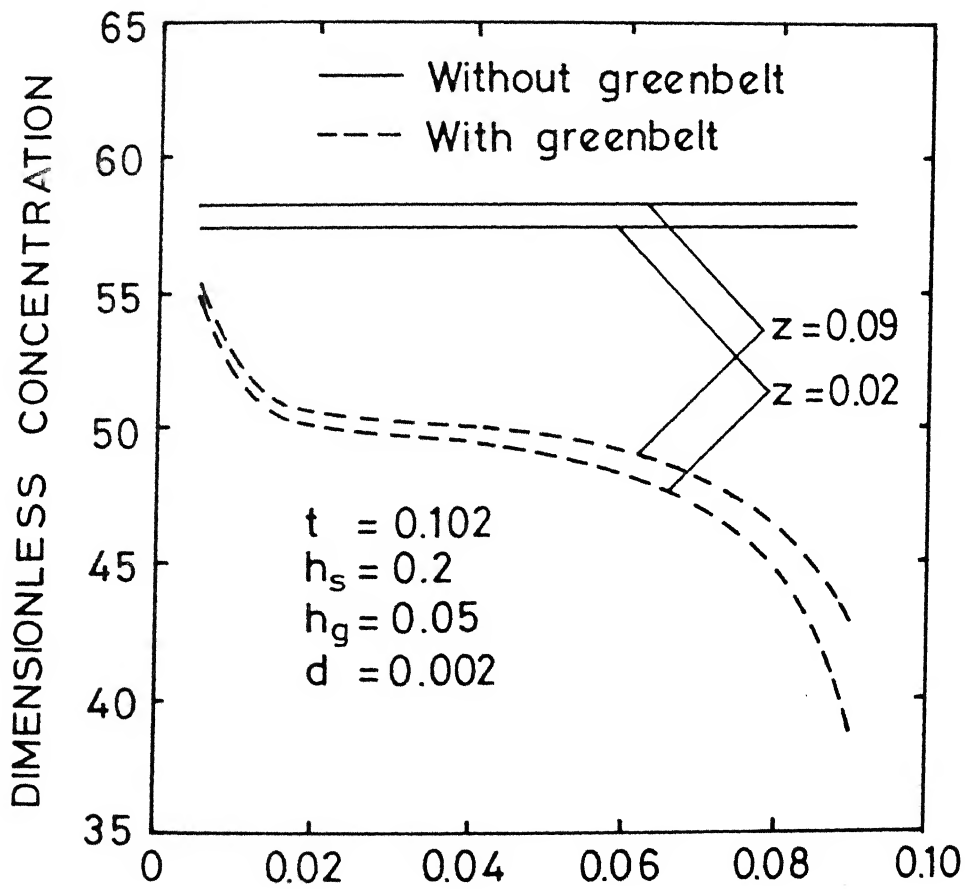
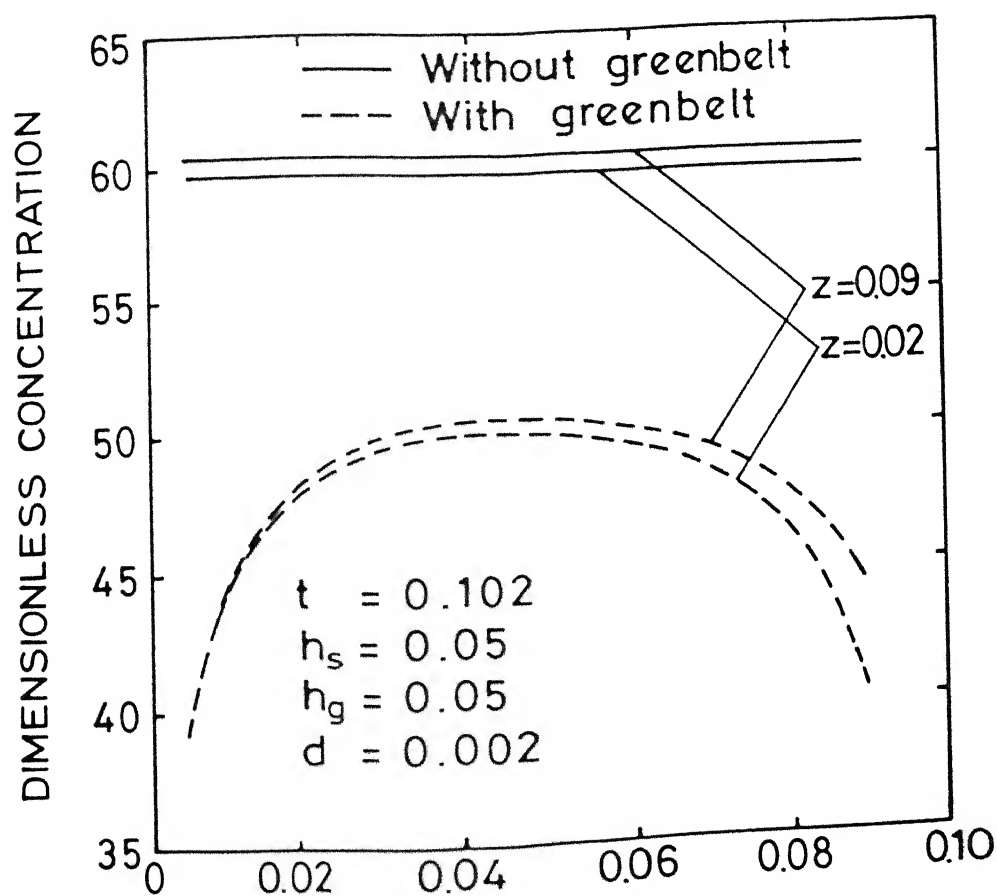
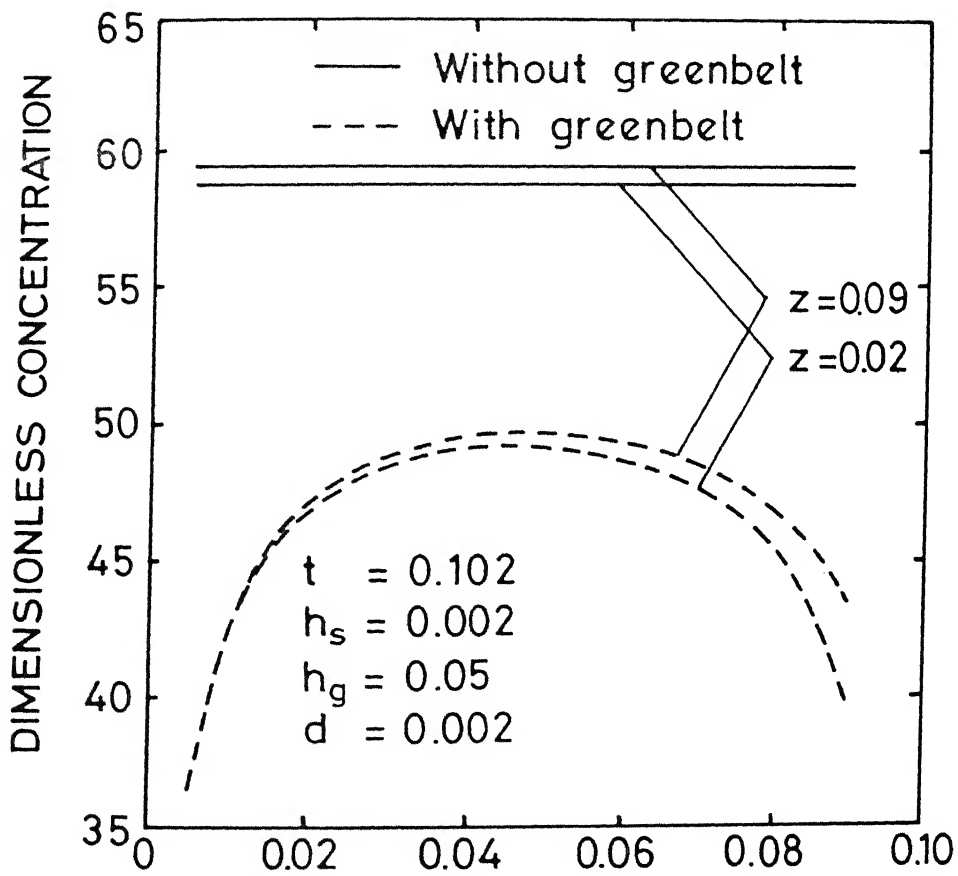


FIG.4.2 CONCENTRATION DISTRIBUTION AT  $x = 0.1$  (RECEPTOR) FOR  $h_s > h_g$ , WHEN FLUX IS INSTANTANEOUS.



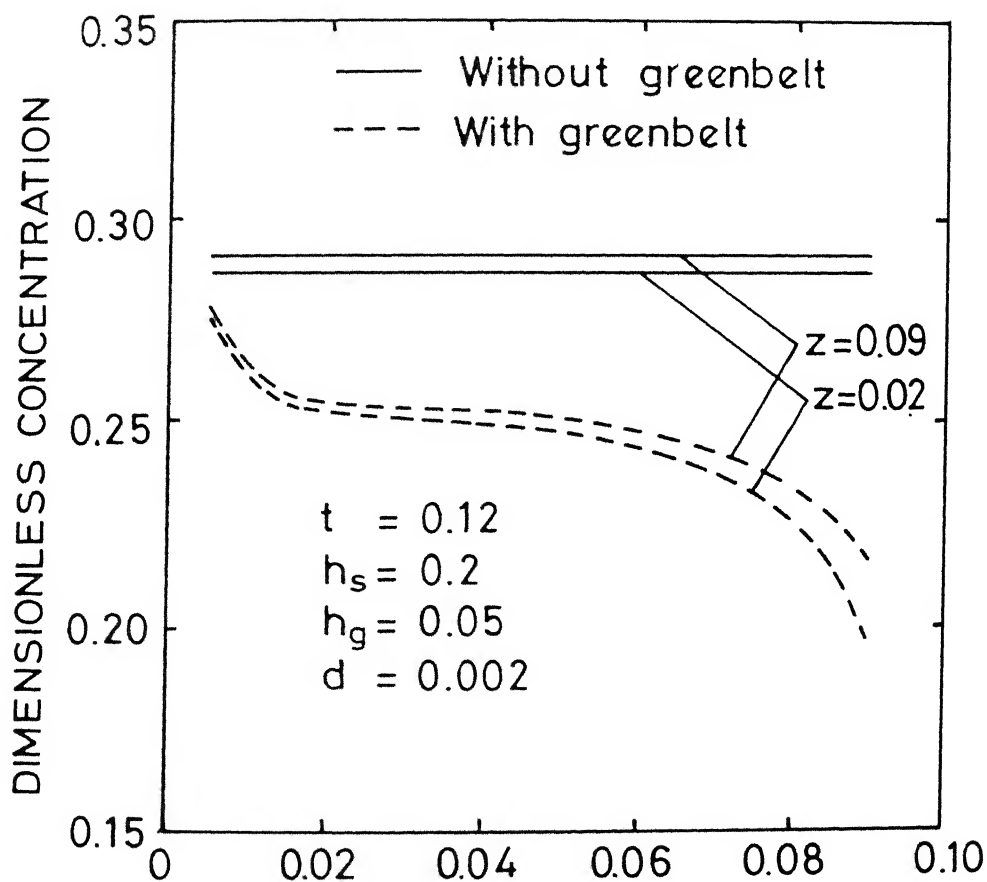
DIMENSIONLESS DISTANCE OF GREENBELT FROM THE SURFACE ( $x_1$ )

FIG.4.3 CONCENTRATION DISTRIBUTION AT  $x=0.1$  (RECEIVER) FOR  $h_s = h_g$ , WHEN FLUX IS INSTANTANEOUS.



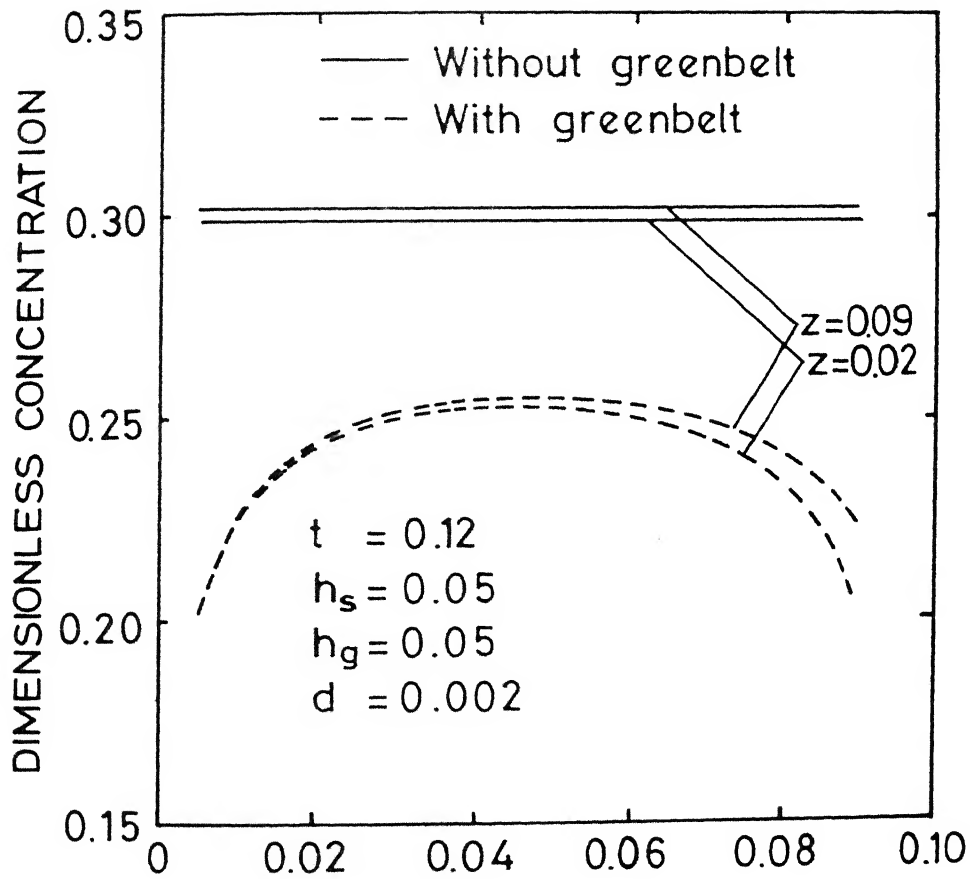
DIMENSIONLESS DISTANCE OF GREENBELT FROM THE SOURCE ( $x_1$ )  
 FIG. 4.4 CONCENTRATION DISTRIBUTION AT  $x=0.1$  (RECEPTOR) FOR  
 $h_s < h_g$ , WHEN FLUX IS INSTANTANEOUS.





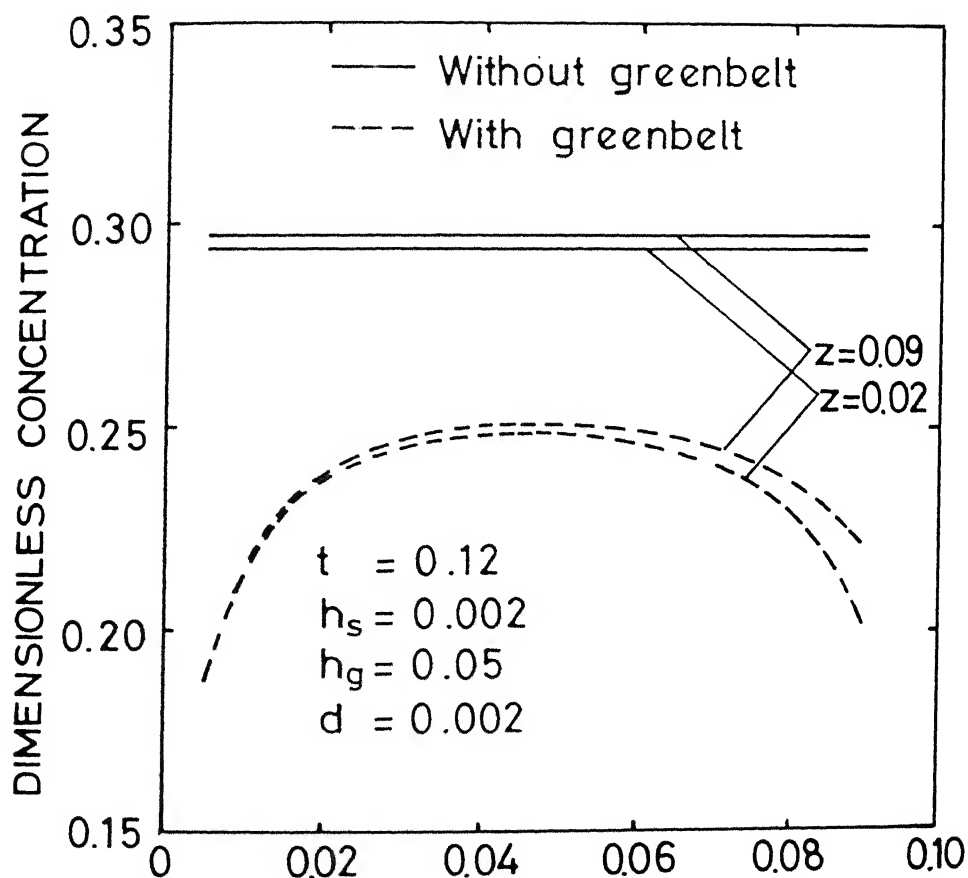
DIMENSIONLESS DISTANCE OF GREENBELT FROM THE SOURCE ( $x_l$ )

FIG.4.5 CONCENTRATION DISTRIBUTION AT  $x=0.1$  (RECEPTOR) FOR  $h_s > h_g$ , WHEN FLUX IS CONSTANT.



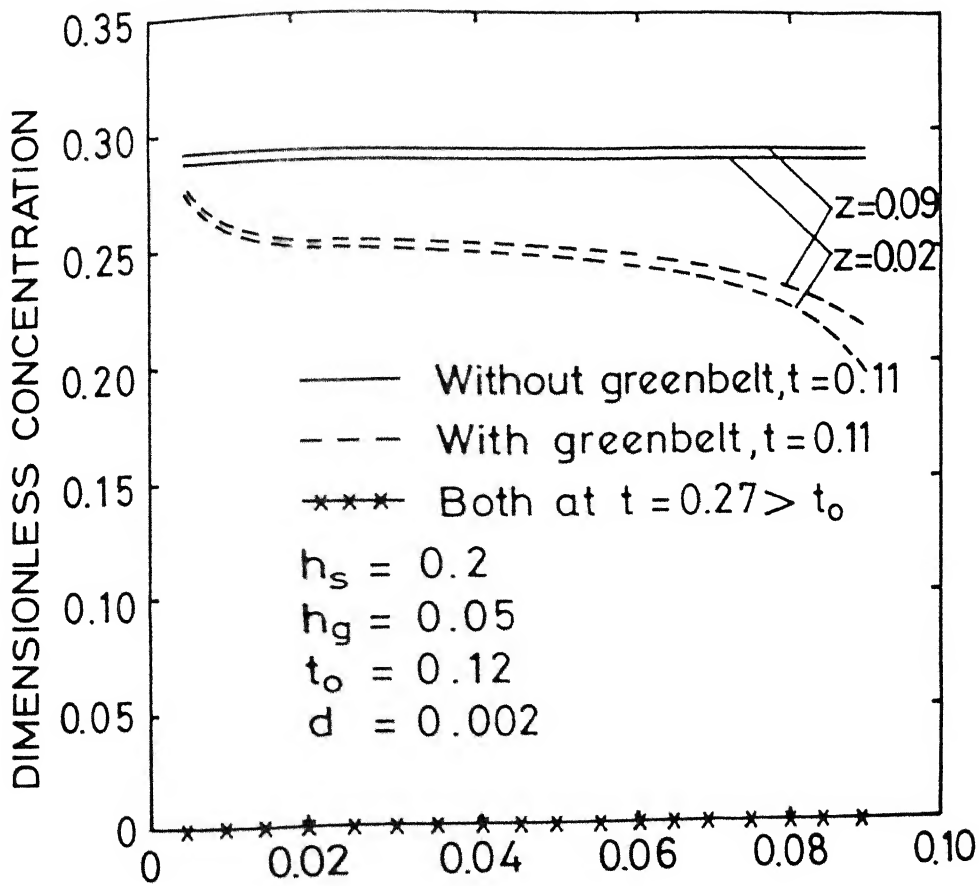
DIMENSIONLESS DISTANCE OF GREENBELT FROM THE SOURCE ( $x_1$ )

FIG.4.6 CONCENTRATION DISTRIBUTION AT  $x=0.1$  (RECEPTOR) FOR  $h_s = h_g$ , WHEN FLUX IS CONSTANT.



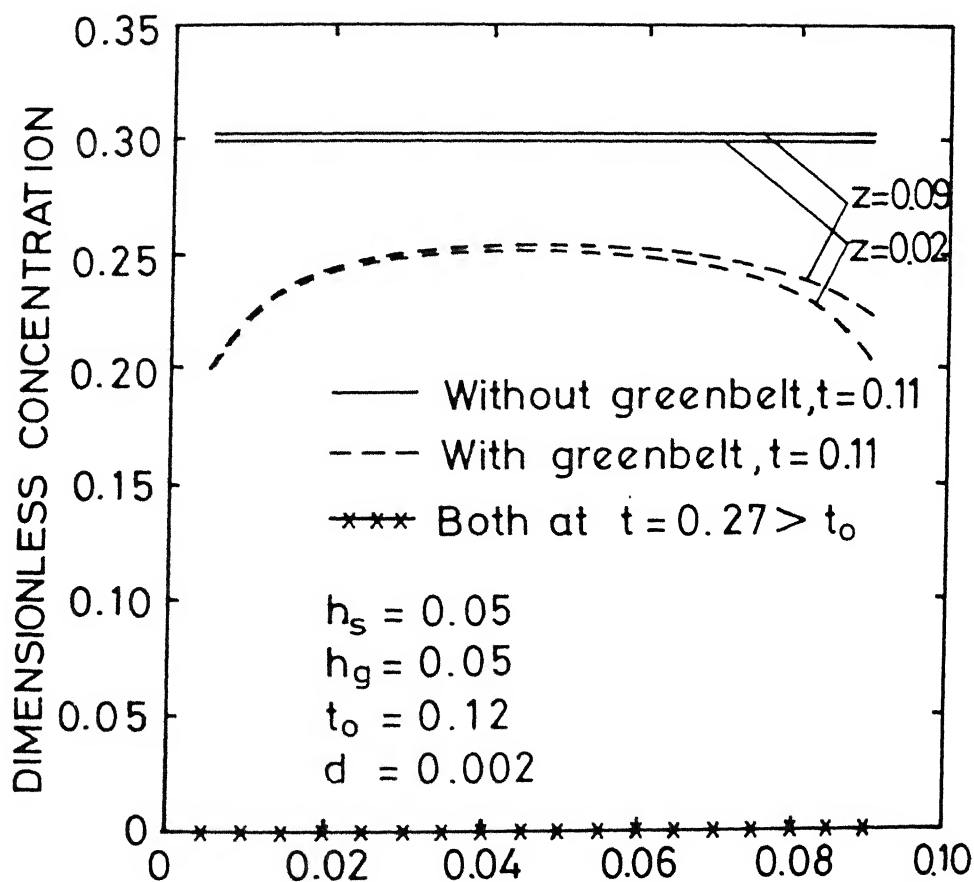
DIMENSIONLESS DISTANCE OF GREENBELT FROM THE SOURCE ( $x_1$ )

FIG.4.7 CONCENTRATION DISTRIBUTION AT  $x = 0.1$  (RECEPTOR) FOR  $h_s < h_g$ , WHEN FLUX IS CONSTANT.



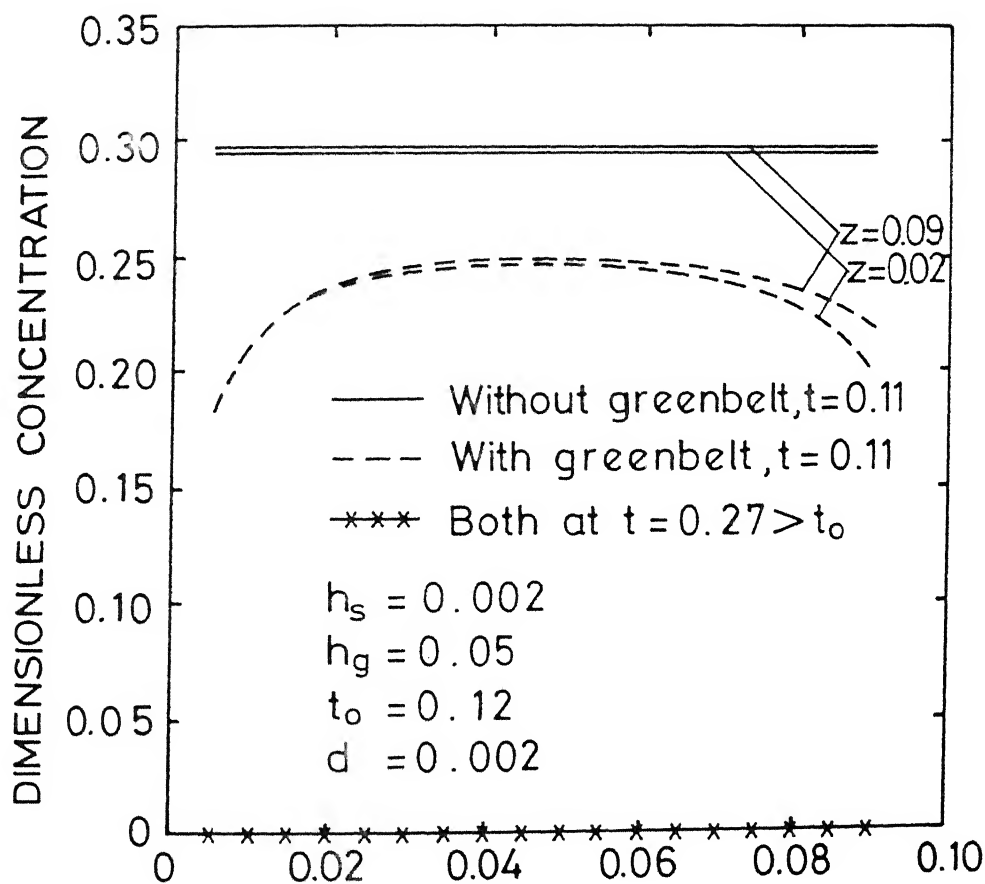
DIMENSIONLESS DISTANCE OF GREENBELT FROM THE SOURCE ( $x_1$ )

FIG. 4.8 CONCENTRATION DISTRIBUTION AT  $x=0.1$  (RECEPTOR) FOR  $h_s > h_g$ , WHEN FLUX IS STEP FUNCTION TYPE.



DIMENSIONLESS DISTANCE OF GREENBELT FROM THE SOURCE( $x$ )

FIG.4.9 CONCENTRATION DISTRIBUTION AT  $x=0.1$  ( RECEPTOR )  
 FOR  $h_s = h_g$  , WHEN FLUX IS STEP FUNCTION TYPE .



DIMENSIONLESS DISTANCE OF GREENBELT FROM THE SOURCE( $x_1$ )

FIG.4.10 CONCENTRATION DISTRIBUTION AT  $x=0.1$  (RECEPTOR) FOR  $h_s < h_g$ , WHEN FLUX IS STEP FUNCTION TYPE.

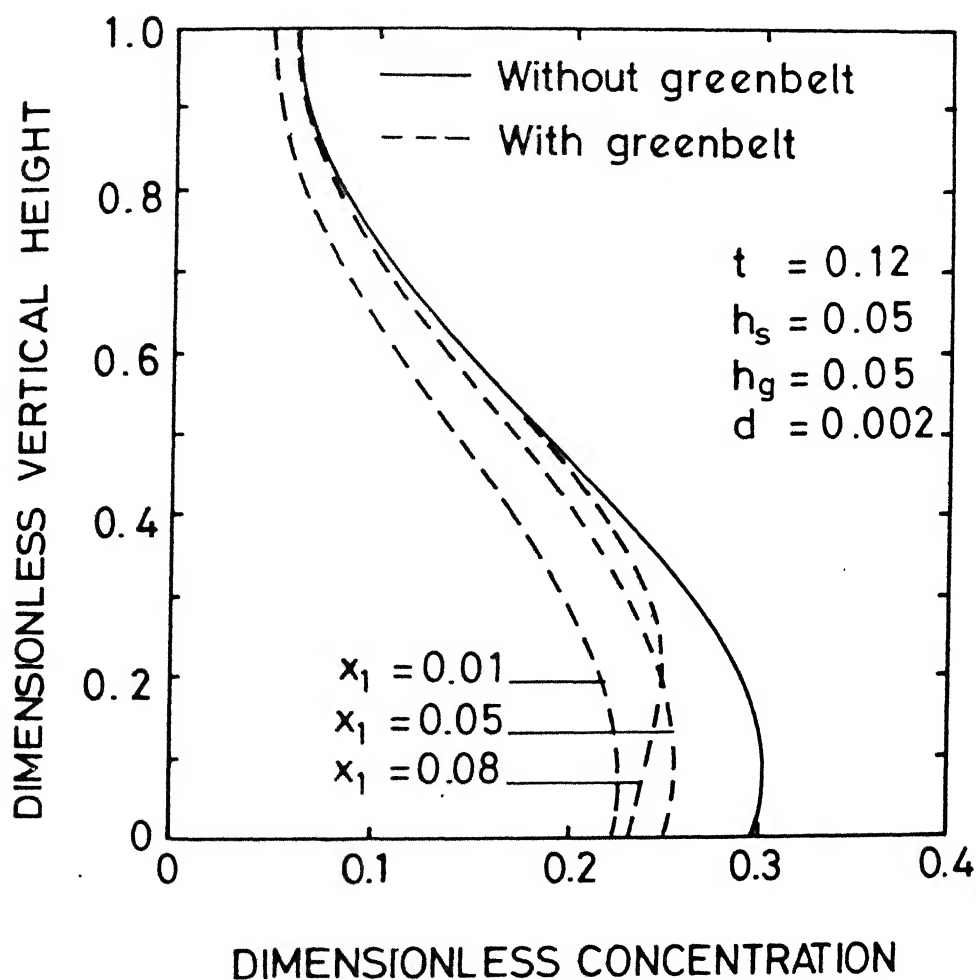


FIG.4.12 VERTICAL CONCENTRATION PROFILES AT  $x = 0.1$  (RECEPTOR) FOR  $h_s = h_g$ , WHEN FLUX IS CONSTANT.

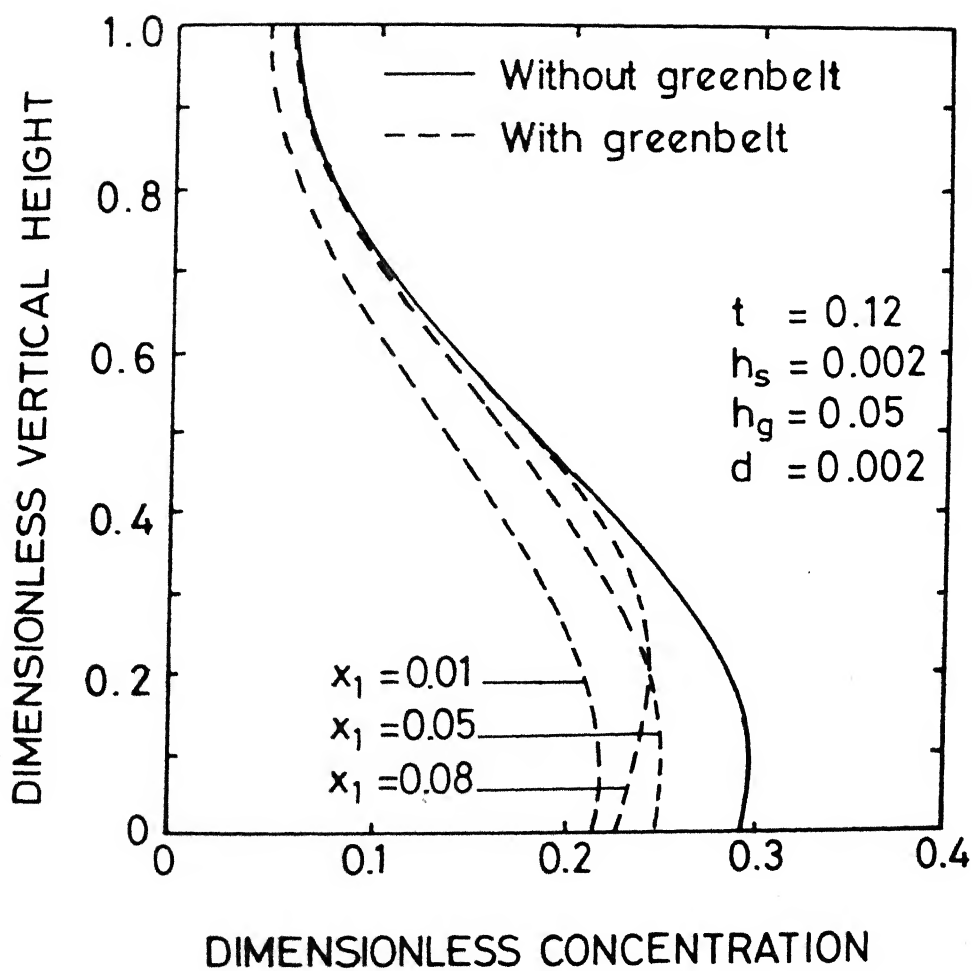


FIG. 4.13 VERTICAL CONCENTRATION PROFILES AT  $x = 0.1$  (RECEPTOR) FOR  $h_s < h_g$ , WHEN FLUX IS CONSTANT.



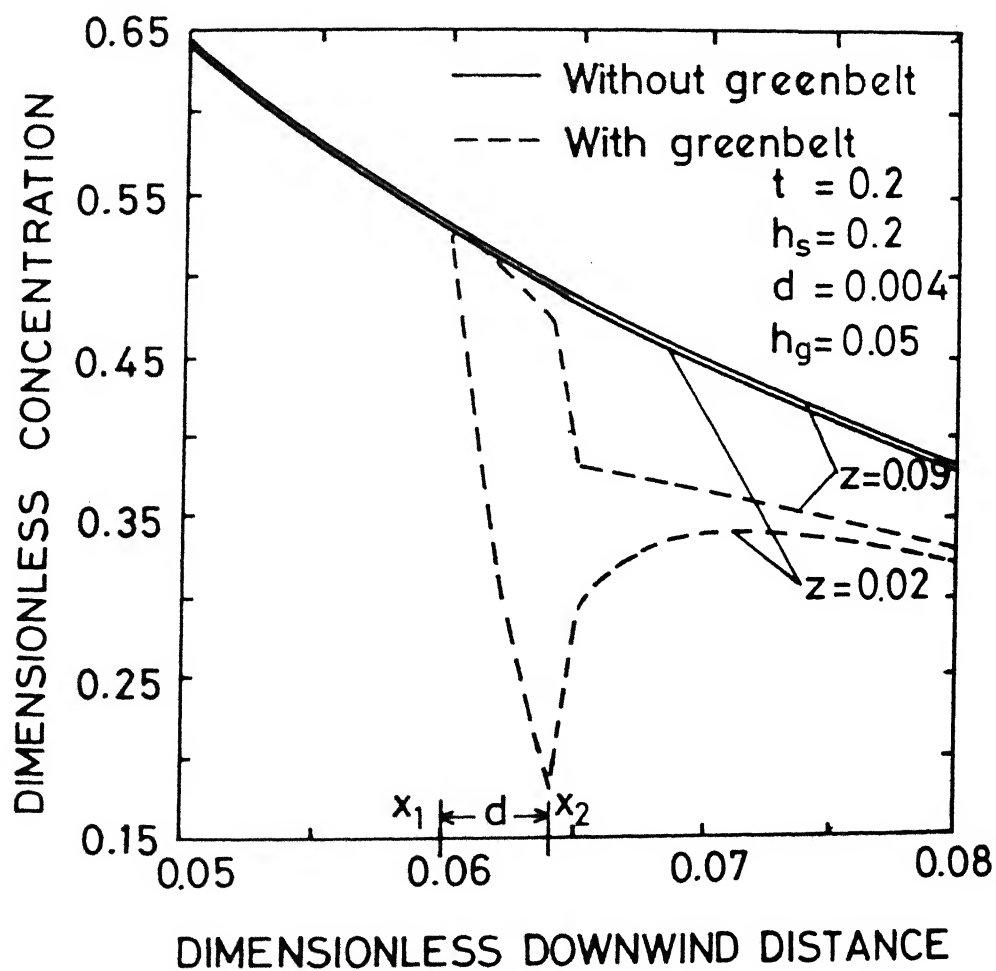


FIG. 4.14 CONCENTRATION DECREASE IN GREENBELT FOR CONSTANT FLUX.

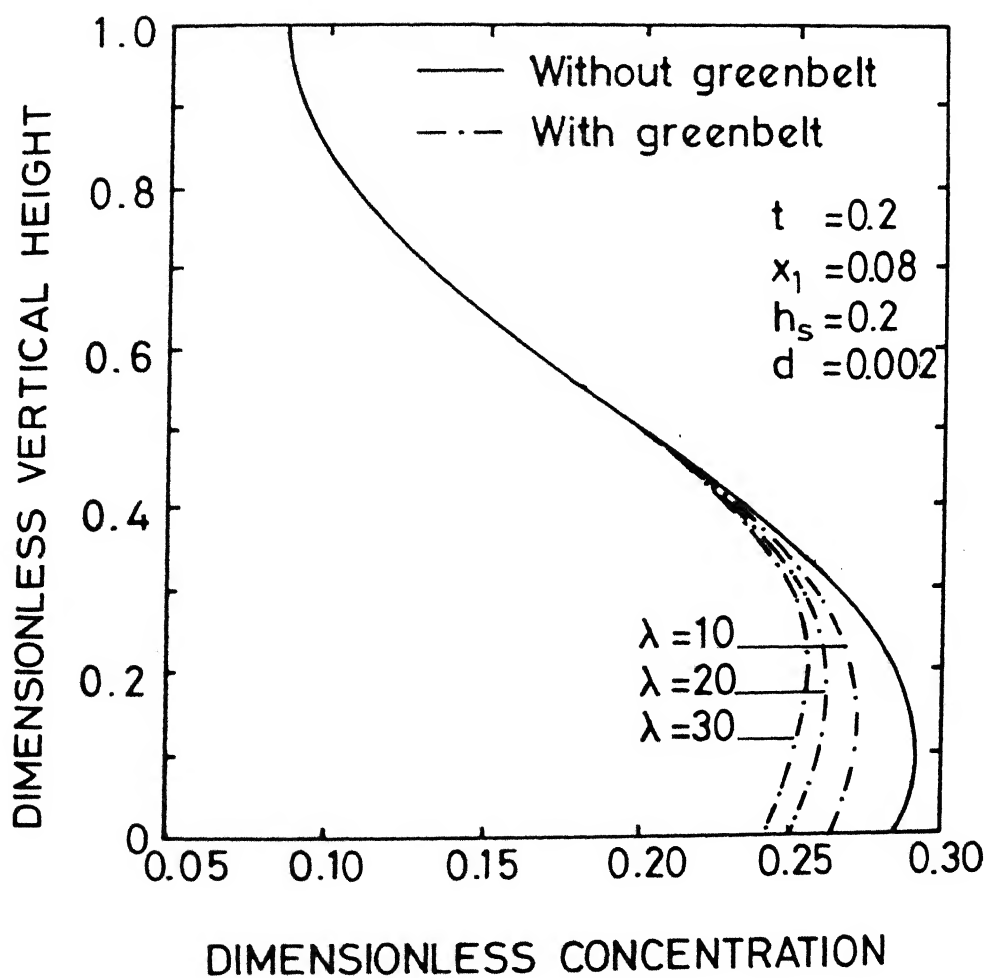


FIG.4.15 EFFECT OF  $\lambda$  ON CONCENTRATION DISTRIBUTION  
AT  $x = 0.1$  (RECEPTOR)

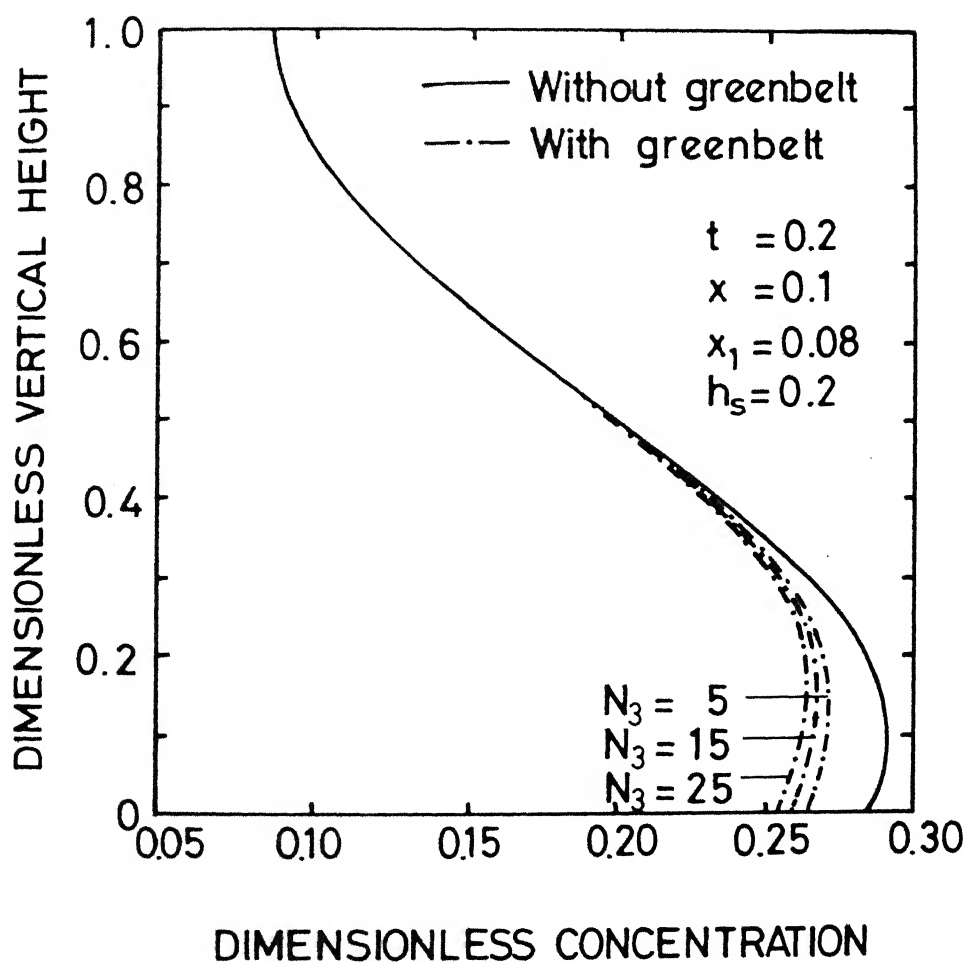


FIG.4.16 EFFECT OF  $N_3$ , THE DEPOSITION VELOCITY AT THE TOP OF THE GREENBELT, ON CONCENTRATION DISTRIBUTION AT  $x = 0.1$  (RECEPTOR)

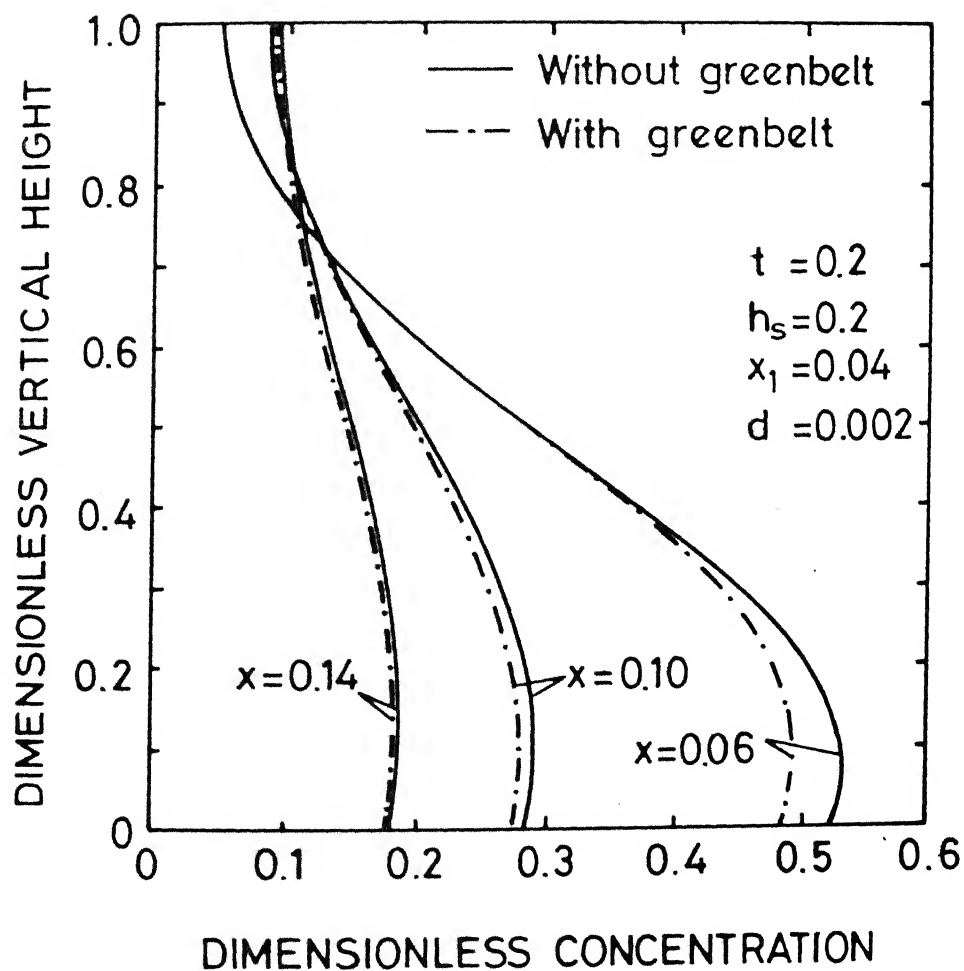
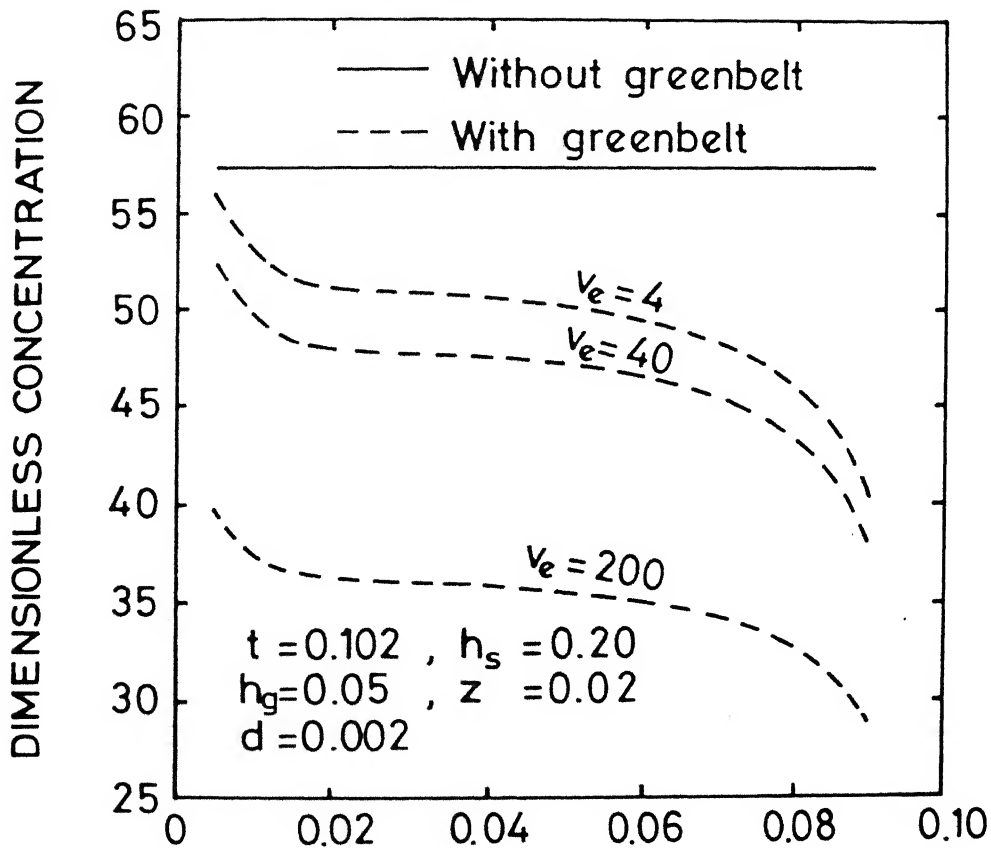
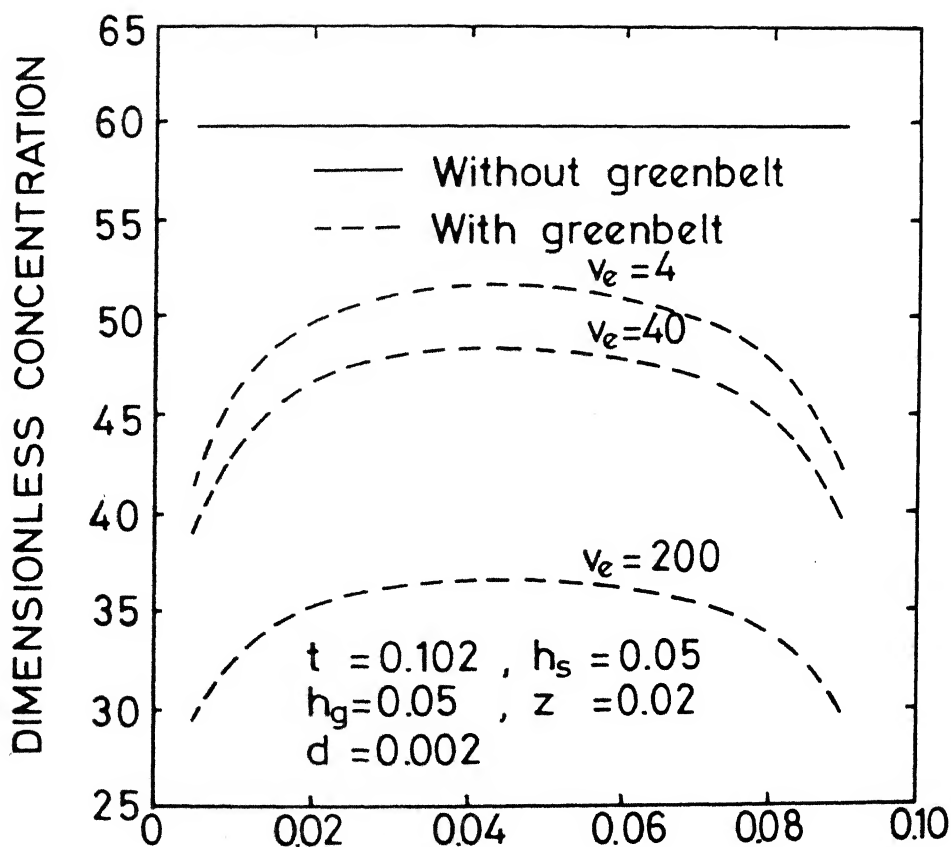


FIG.4.17 EFFECT OF INCREASING RECEPTOR LOCATION FROM THE GREENBELT AT  $x_1 = 0.04$ .



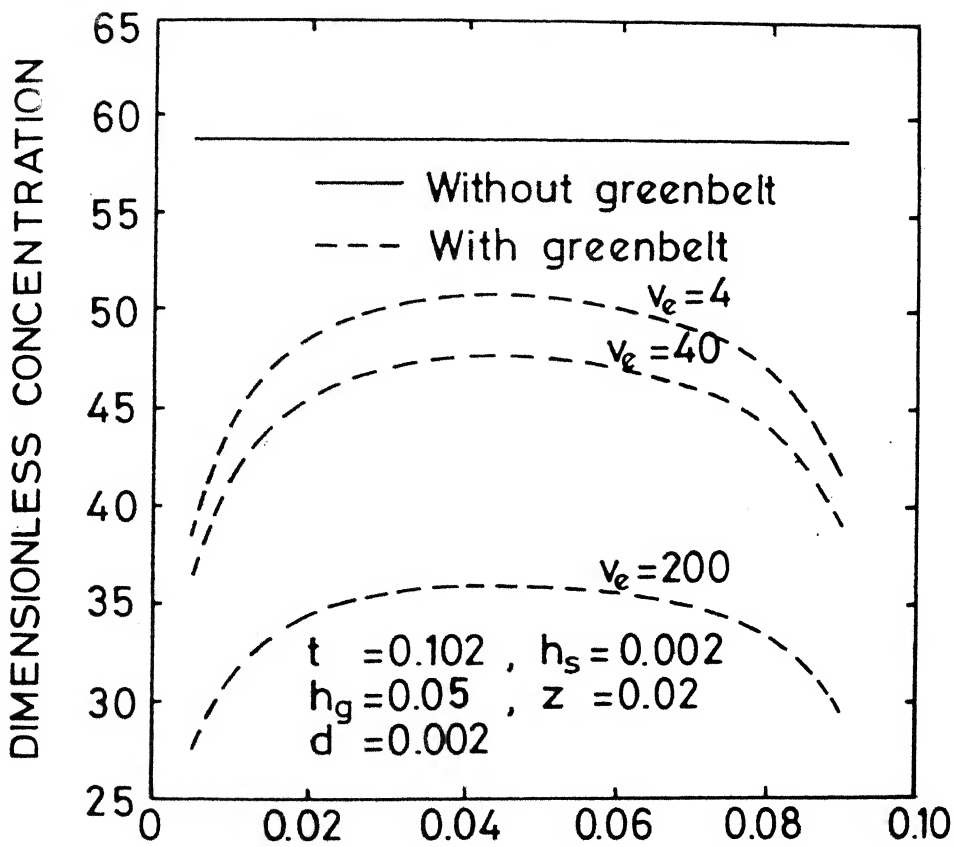
DIMENSIONLESS DISTANCE OF GREENBELT FROM THE SOURCE ( $x_1$ )

FIG.4.18 CONCENTRATION DISTRIBUTION AT  $x=0.1$  (RECEPTOR) FOR  $h_s > h_g$ , WHEN FLUX IS INSTANTANEOUS.



DIMENSIONLESS DISTANCE OF GREENBELT FROM THE SOURCE ( $x_p$ )

FIG.4.19 CONCENTRATION DISTRIBUTION AT  $x = 0.1$  (RECEPTOR) FOR  $h_s = h_g$ , WHEN FLUX IS INSTANTANEOUS.



DIMENSIONLESS DISTANCE OF GREENBELT FROM THE SOURCE ( $x_1$ )

FIG.4.20 CONCENTRATION DISTRIBUTION AT  $x = 0.1$  (RECEPTOR) FOR  $h_s < h_g$  , WHEN FLUX IS INSTANTANEOUS.

## CHAPTER V

# EFFECT OF PRECIPITATION SCAVENGING ON DISPERSION OF AIR POLLUTANT IN THE ATMOSPHERE

### 5.0 INTRODUCTION

The study of various kinds of removal mechanisms which occur in the environment such as scavenging by rain droplets, wet and dry deposition of both particulate and gaseous pollutants is very important in view of the fact that our environment is continuously stressed by different kinds of air pollutants/toxicants emitted from different sources. One such important mechanism for removal of pollutants from the atmosphere is due to precipitation scavenging, a process useful in cleaning the environment of polluted cities in India during monsoon season. The study of scavenging of pollutant by precipitation has received considerable attention during the last few decades, e.g., Hales(1972,1989), Hales *et al.*(1973), Slinn(1974,1977), Peters(1976), Hill and Adamowicz(1977), Adamowicz(1979), Overton *et al.*(1979), Fisher(1982), Scott(1982a,b), Levine and Schwartz(1982), Shukla *et al.*(1982), Chang(1984), Kumar(1985,1986,1989), Shukla and Chauhan(1987), Luecken *et al.*(1989). In particular, Hales(1972) presented some fundamentals for the general analysis of atmospheric gas scavenging by rain and pointed out that the process of trace gas scavenging is reversible in nature and phenomenon of absorption and desorption may cause a redistribution of pollutants in the atmosphere. A simpler linearized model for predicting the washout of gaseous constituents from industrial



plumes by taking into account the reversibility of adsorption process has been presented by Hales *et al.* (1973) assuming the rain to be composed of spherical, non-interacting drops of static size distribution. An analytical study for the redistribution of gas plume caused by reversible washout has been investigated by Slinn (1974). The problem of irreversible scavenging for  $\text{HNO}_3$  vapor and calculation of washout coefficients for removal of  $\text{HNO}_3$  from the atmosphere has been considered by Levine and Schwartz (1982). Kumar (1985) studied the simultaneous process of trace gas removal from the atmosphere and absorption of these gases in rain drops using an Eulerian model but his model does not take into account the wind velocity and presence of a time dependent source.

In the present investigation we, therefore, study the effect of precipitation scavenging on the unsteady state dispersion of a reactive air pollutant emitted from a time dependent point source, assuming the uniform distribution of rain droplets in the atmosphere which absorb the pollutant and remove it by their fall on the ground with a constant velocity. We consider that the concentration of the pollutant in the gaseous phase is governed by the unsteady state three dimensional convective diffusion equation with removal terms while the concentration of the absorb pollutant in the droplets is governed by a simplified equation which neglects diffusion term but takes into account the falling of rain droplets on the ground. These equations are then solved using appropriate initial and boundary conditions to study the effect of precipitation scavenging on the dispersion of pollutant in the atmosphere.

analysis are: (i) Instantaneous, and (ii) Constant.

### 5.1 MATHEMATICAL MODEL

Consider the unsteady state dispersion of a reactive air pollutant emitted from a time dependent point source of strength  $Q(t)$  located at height  $h_s$  and the washout takes place below the cloud base situated at height  $z = H$ . Here we consider two phases in the atmosphere viz., the pollutant in the gaseous phase and absorbed pollutant phase in the droplets.

The differential equations governing the concentration  $C(x,y,z,t)$  of the pollutant in the gaseous phase is written as,

$$\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} = K_y \frac{\partial^2 C}{\partial y^2} + K_z \frac{\partial^2 C}{\partial z^2} - (k + k_g)C + \nu C_a \quad (5.1)$$

where  $x, y, z$  are cartesian co-ordinates,  $t$  is the time,  $x$ -axis is taken along the wind direction,  $z$ -axis vertically upwards,  $U$  is the mean wind velocity,  $K_y$  and  $K_z$  are diffusivities in  $y$  and  $z$  directions respectively,  $k$  is the first order removal rate coefficient of the pollutant due to some natural mechanism and  $k_g$  is the depletion rate coefficient due to precipitation scavenging by rain which is zero if there is no rain and  $\nu$  is the coefficient of rate of desorption of the absorbed pollutant  $C_a$  in the droplet phase.

We prescribe the following initial and boundary conditions for equation (5.1),

$$C(x,y,z,t) = 0 \quad \text{at } t = 0 \quad (5.2)$$

$$C(x,y,z,t) = \frac{Q(t)}{U} \delta(y) \delta(z-h_s) \quad \text{at } x = 0 \quad (5.3)$$

$$(5.4)$$

$$K_z \frac{\partial C}{\partial z} = v_d C \quad \text{at } z = 0 \quad (5.5)$$

$$\frac{\partial C}{\partial z} = 0 \quad \text{at } z = H \quad (5.6)$$

The following forms of time dependent flux  $Q(t)$  at the point source are considered in the analysis,

$$(i) \text{ Flux is Instantaneous, } Q(t) = Q_0 \delta(t) \quad (5.7)$$

$$(ii) \text{ Flux is Constant, } Q(t) = Q_c \quad (5.8)$$

Now we proceed to write the equation governing the concentration of the absorbed pollutant in the droplet phase. Since the concentration of the absorbed pollutant in the droplets is directly influenced by the concentration of the pollutant in the gaseous phase, it is necessary to consider simultaneously the coupled process of pollutant depletion in gaseous phase and absorption in the droplet phase of the pollutant species, (Kumar, 1985).

The equation governing the concentration  $C_a(x,y,z,t)$  of the absorbed pollutant in the droplet phase is written as,

$$\frac{\partial C_a}{\partial t} - w(r) \frac{\partial C_a}{\partial z} = \gamma C - \eta C_a \quad (5.9)$$

with initial and boundary conditions as follows,

$$C_a(x,y,z,t) = 0 \quad \text{at } t = 0 \quad (5.10)$$

$$C_a(x,y,z,t) = 0 \quad \text{at } z = H \quad (5.11)$$

where  $w$  is the terminal velocity of rain droplets falling on the ground, which depends on its radius  $r$  but in the following analysis we assume the terminal velocity as constant and rain droplets to be uniformly distributed. The absorption rate

removal rate coefficient, are also assumed to be constant.

In equation (5.1)  $\nu C_a$  represents the source term due to desorption of the absorbed pollutant. It may be noted that  $\nu \leq \eta$  and  $\nu/k_g \ll 1$ , therefore, we neglect the desorption of the absorbed pollutant (i.e.,  $\nu C_a$  is assumed negligible).

Introduce the following dimensionless quantities,

$$\begin{aligned}\bar{t} &= \frac{K_z t}{H^2}, \quad \bar{x} = \frac{K_z x}{U H^2}, \quad \bar{y} = \frac{y}{H}, \quad \bar{z} = \frac{z}{H}, \quad \bar{h}_s = \frac{h_s}{H} \\ \bar{C} &= \frac{U H^2}{Q_c} C, \quad \bar{C}_a = \frac{U H^2}{Q_c} C_a, \quad \bar{Q}(t) = \frac{Q(t)}{Q_c}, \quad \bar{Q}_0 = \frac{Q_0}{Q_c} \frac{K_z}{H^2} \\ \bar{w} &= \frac{H w}{K_z}, \quad \bar{\gamma} = \frac{H^2 \gamma}{K_z}, \quad \bar{\eta} = \frac{H^2 \eta}{K_z}\end{aligned}$$

The system of equations (5.1-5.11) can be written in dimensionless form as, (dropping bars for convenience)

$$\frac{\partial C}{\partial t} + \frac{\partial C}{\partial x} = \beta \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} - (\alpha + \alpha_g) C \quad (5.12)$$

$$C(x, y, z, t) = 0 \quad \text{at} \quad t = 0 \quad (5.13)$$

$$C(x, y, z, t) = Q(t) \delta(y) \delta(z - h_s) \quad \text{at} \quad x = 0 \quad (5.14)$$

$$C(x, y, z, t) = 0 \quad \text{as} \quad y \rightarrow \pm \infty \quad (5.15)$$

$$\frac{\partial C}{\partial z} = N C \quad \text{at} \quad z = 0 \quad (5.16)$$

$$\frac{\partial C}{\partial z} = 0 \quad \text{at} \quad z = 1 \quad (5.17)$$

$$\frac{\partial C_a}{\partial t} - w \frac{\partial C_a}{\partial z} = \gamma C - \eta C_a \quad (5.18)$$

$$C_a(x, y, z, t) = 0 \quad \text{at} \quad t = 0 \quad (5.19)$$

$$C_a(x, y, z, t) = 0 \quad \text{at} \quad z = 1 \quad (5.20)$$

$$\text{where } \alpha = \frac{H^2 k}{K_z}, \quad \alpha_g = \frac{H^2 k_g}{K_z}, \quad \beta = \frac{K_y}{K_z}, \quad N = \frac{v_d H}{K_z}$$

and

$$(i) \text{ Flux is Instantaneous, } Q(t) = Q_0 \delta(t) \quad (5.21)$$

$$(ii) \text{ Flux is Constant, } Q(t) = 1 \quad (5.22)$$

## 5.2 CONCENTRATION DISTRIBUTIONS

The solutions for concentration distribution of pollutant,  $C$  and  $C_a$  are obtained by solving equations (5.12) - (5.20) and written in each cases as follows,

### 5.2.1 CASE I WHEN FLUX IS INSTANTANEOUS AT THE SOURCE

$$C(x, y, z, t) = Q_0 \frac{e^{-y^2/4\beta x}}{\sqrt{4\pi\beta x}} \sum_{n=1}^{\infty} \exp\left(-(\alpha + \alpha_g + \lambda_n^2)x\right) \frac{F_n(h_s)}{P_n} F_n(z) \delta(t-x) \quad (5.23)$$

$$C_a(x, y, z, t) = Q_0 \gamma \frac{e^{-y^2/4\beta x}}{\sqrt{4\pi\beta x}} \sum_{n=1}^{\infty} \exp\left(-(\alpha + \alpha_g + \lambda_n^2)x\right) \frac{F_n(h_s)}{P_n} f_n(x, z, t) \quad (5.24)$$

where

$$F_n(z) = \cos \lambda_n z + \frac{N}{\lambda_n} \sin \lambda_n z$$

$$P_n = \int_0^1 (\cos \lambda_n z + \frac{N}{\lambda_n} \sin \lambda_n z)^2 dz$$

$\lambda_n^s$  are the roots of the following transcendental equation

$$\lambda_n \tan \lambda_n = N, \quad n = 1, 2, 3, \dots$$

$$\begin{aligned} f_n(x, z, t) = & -f_{n1}(x, z, t) \left( \cos \lambda_n + N \frac{\sin \lambda_n}{\lambda_n} \right) \\ & + f_{n2}(x, z, t) \left( -N \cos \lambda_n + \lambda_n \sin \lambda_n \right) \\ & + f_{n3}(x, z, t) \left( \cos \lambda_n z + N \frac{\sin \lambda_n z}{\lambda_n} \right) \\ & + f_{n4}(x, z, t) \left( N \cos \lambda_n z - \lambda_n \sin \lambda_n z \right) \end{aligned}$$

$$f_{n1}(x, z, t) = e^{-\eta(t-x)} \cos\left(\lambda_n w(t-x - \frac{1-z}{w})\right) H\left(t - x - \frac{1-z}{w}\right) H\left(t - \frac{1-z}{w}\right)$$

$$f_{n2}(x, z, t) = \frac{1}{\lambda_n} e^{-\eta(t-x)} \sin\left(\lambda_n w(t-x - \frac{1-z}{w})\right) H\left(t - x - \frac{1-z}{w}\right) H\left(t - \frac{1-z}{w}\right)$$

$$f_{n3}(x, z, t) = e^{-\eta(t-x)} \cos\left(\lambda_n w(t-x)\right) H(t-x)$$

$$f_{n4}(x, z, t) = \frac{1}{\lambda_n} e^{-\eta(t-x)} \sin\left(\lambda_n w(t-x)\right) H(t-x)$$

and  $\delta(t-x)$  is the Dirac delta function defined as, (Carslaw and Jaeger, 1941)

$$\begin{aligned} \delta(t-x) &= 0, \quad t < x \\ &= 1/\epsilon, \quad x \leq t \leq x+\epsilon \\ &= 0, \quad t > x+\epsilon \end{aligned}$$

### 5.2.2 CASE II WHEN FLUX IS CONSTANT AT THE SOURCE

$$C(x, y, z, t) = \frac{e^{-y^2/4\beta x}}{\sqrt{4\pi\beta x}} \sum_{n=1}^{\infty} \exp\left(-(\alpha + \alpha_g + \lambda_n^2)x\right) \frac{F_n(h_s)}{P_n} F_n(z) H(t-x) \quad (5.25)$$

$$C_a(x, y, z, t) = \gamma \frac{e^{-y^2/4\beta x}}{\sqrt{4\pi\beta x}} \sum_{n=1}^{\infty} \exp\left(-(\alpha + \alpha_g + \lambda_n^2)x\right) \frac{F_n(h_s)}{P_n} F_n(z) g_n(x, z, t) \quad (5.26)$$

where

$$\begin{aligned} g_n(x, z, t) &= -g_{n1}(x, z, t) \left( \cos \lambda_n + N \frac{\sin \lambda_n}{\lambda_n} \right) \\ &+ g_{n2}(x, z, t) \left( -N \cos \lambda_n + \lambda_n \sin \lambda_n \right) \\ &+ g_{n3}(x, z, t) \left( \cos \lambda_n z + N \frac{\sin \lambda_n z}{\lambda_n} \right) \\ &+ g_{n4}(x, z, t) \left( N \cos \lambda_n z - \lambda_n \sin \lambda_n z \right) \end{aligned}$$

$$g_{n1}(x, z, t) = \left( \frac{e^{-\eta(t-x)} \left( -\eta \cos(\arg 1) + \lambda_n w \sin(\arg 1) \right) + \eta e^{-\frac{\eta(1-z)}{w}}}{\eta^2 + \lambda_n^2 w^2} \right) \times H\left(t - x - \frac{1-z}{w}\right) H\left(t - \frac{1-z}{w}\right)$$

$$g_{n2}(x, z, t) = \frac{1}{\lambda_n} \left( \frac{e^{-\eta(t-x)} \left( -\eta \sin(\arg 1) - \lambda_n w \cos(\arg 1) \right) + \lambda_n w e^{-\frac{\eta(1-z)}{w}}}{\eta^2 + \lambda_n^2 w^2} \right) \times H\left(t - x - \frac{1-z}{w}\right) H\left(t - \frac{1-z}{w}\right)$$

$$g_{n3}(x, z, t) = \left( \frac{e^{-\eta(t-x)} \left( -\eta \cos(\arg 2) + \lambda_n w \sin(\arg 2) \right) + \eta}{\eta^2 + \lambda_n^2 w^2} \right) H(t-x)$$

$$g_{n4}(x, z, t) = \frac{1}{\lambda_n} \left( \frac{e^{-\eta(t-x)} \left( -\eta \sin(\arg 2) - \lambda_n w \cos(\arg 2) \right) + \lambda_n w}{\eta^2 + \lambda_n^2 w^2} \right) H(t-x)$$

$$\arg 1 = \lambda_n w \left( t - x - \frac{1-z}{w} \right), \quad \arg 2 = \lambda_n w (t - x)$$

and  $H(t-x)$  is the Heaviside function defined as, (Carslaw and Jaeger, 1941).

$$\begin{aligned} H(t-x) &= 0, \quad t \leq x \\ &= \frac{t}{x+\epsilon}, \quad x < t < x+\epsilon \\ &= 1, \quad t \geq x+\epsilon \end{aligned}$$

### 5.3 DISCUSSION AND RESULTS

To study the effect of precipitation scavenging on the dispersion of air pollutant in the atmosphere, the expressions for concentration distribution of the pollutant in the gaseous phase and that of the absorbed pollutant in the droplets phase have been computed and displayed graphically in Figures 5.1-5.6. The dimensionless parameter values used in the computation are  $Q_0 = 1.0$ ,  $\alpha = 2.00$ ,  $\alpha_g = 20.0$ ,  $\beta = 10.0$ ,  $N = 0.04$ ,  $w = 1000$ ,  $h_s = 0.2$ ,

When flux is instantaneous at the source, the central line concentrations of the pollutant in gaseous phase versus downwind distance with and without rain are shown in Figure 5.1 for different values of  $t$ . It is noted that the concentration of the pollutant decreases as time increases in both the cases and the concentration of the pollutant decreases considerably due to precipitation scavenging by rain.

When flux is constant at the source, the central line concentrations of the pollutant in gaseous phase versus downwind distance with and without rain are shown in Figure 5.2 for different values of  $t$ . It is found that the concentration of the pollutant increases with increase in time and reaches its steady state value as  $t \rightarrow \infty$ . It is noted that the concentration of the pollutant reduces considerably in this case also.

The concentration of the absorbed pollutant  $C_a$  in rain droplets along the center line  $(0,0,h_s)$  with downwind distance for both instantaneous and constant source is shown in Figures 5.3 and 5.4 respectively for different values of  $t$ . It is observed that this concentration decreases as time increases for the case of instantaneous flux and increases for the case of constant flux and reaches its steady state value as  $t \rightarrow \infty$ .

In Figure 5.5 the concentrations of the pollutant in gaseous phase with and without rain are plotted with vertical height at a particular time  $t = 0.06$  for three values of  $x = 0.03, 0.04, 0.05$  for the case when flux is constant at the source. The concentration of the pollutant decreases as  $x$  increases at a time  $t > x$ . It is also seen that the concentration of the pollutant



In Figure 5.6 the variation of concentration of the absorbed pollutant in rain droplet phase with vertical height is also depicted for different values of  $x$  at  $t=0.06$ . It is noted that this concentration increases with decrease in height but decreases as  $x$  increases for  $t > x$ .

From the above analysis, it may therefore be concluded that precipitation scavenging helps in cleaning the atmosphere in those regions of the world where precipitation takes place very frequently.

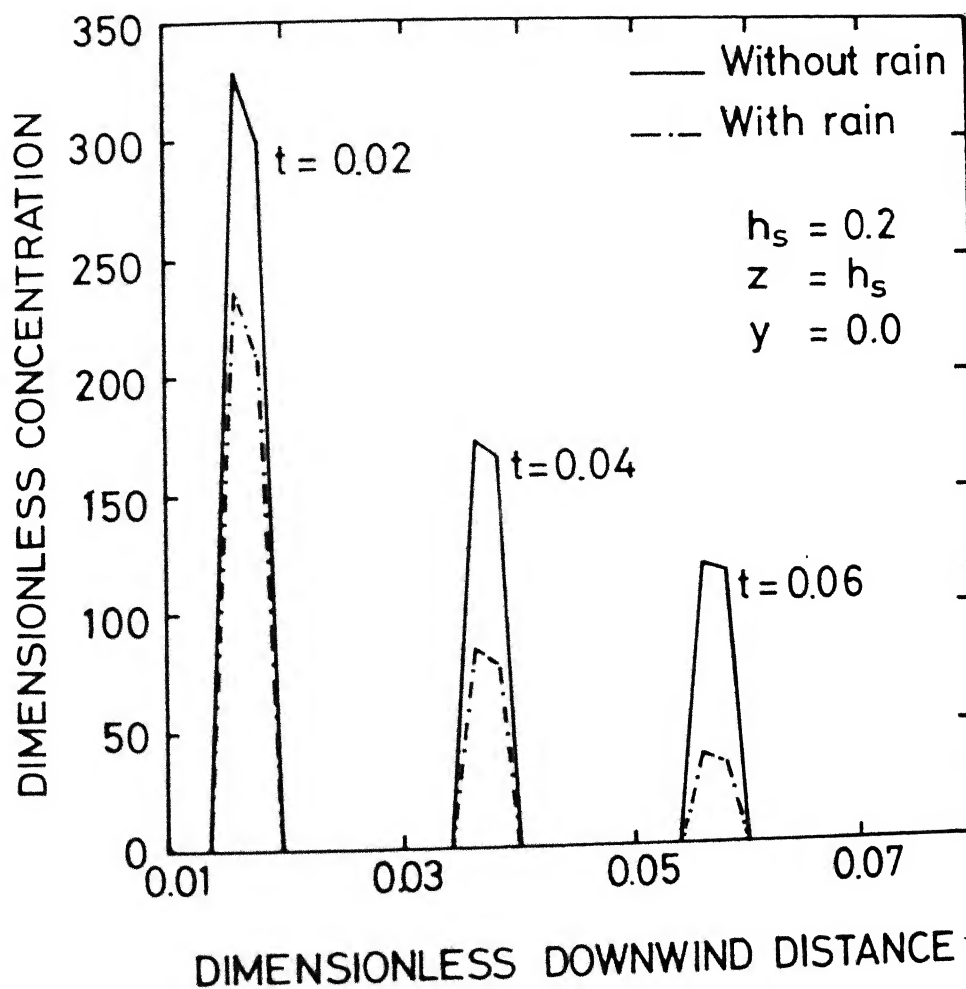


FIG. 5.1 CONCENTRATION-DISTANCE PROFILES IN GASEOUS PHASE FOR INSTANTANEOUS FLUX AT THE SOURCE.

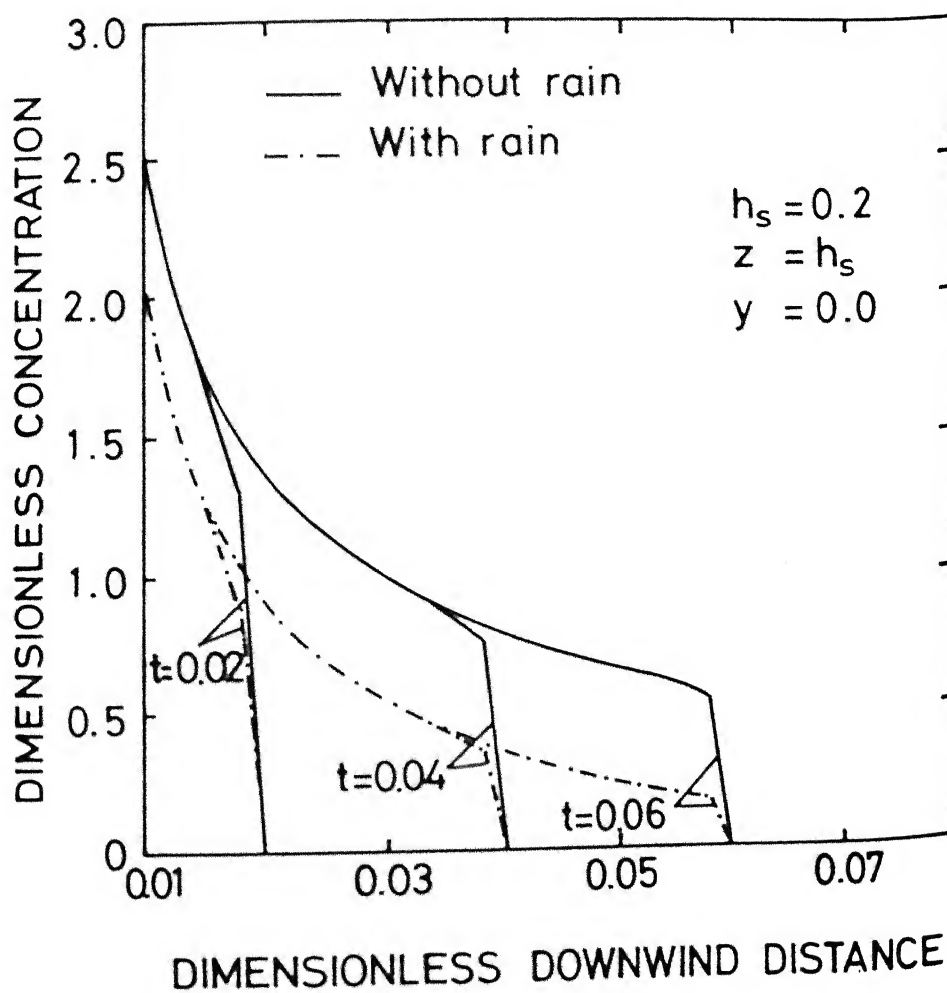


FIG. 5.2 CONCENTRATION-DISTANCE PROFILES IN GASEOUS PHASE FOR CONSTANT FLUX AT THE SOURCE.

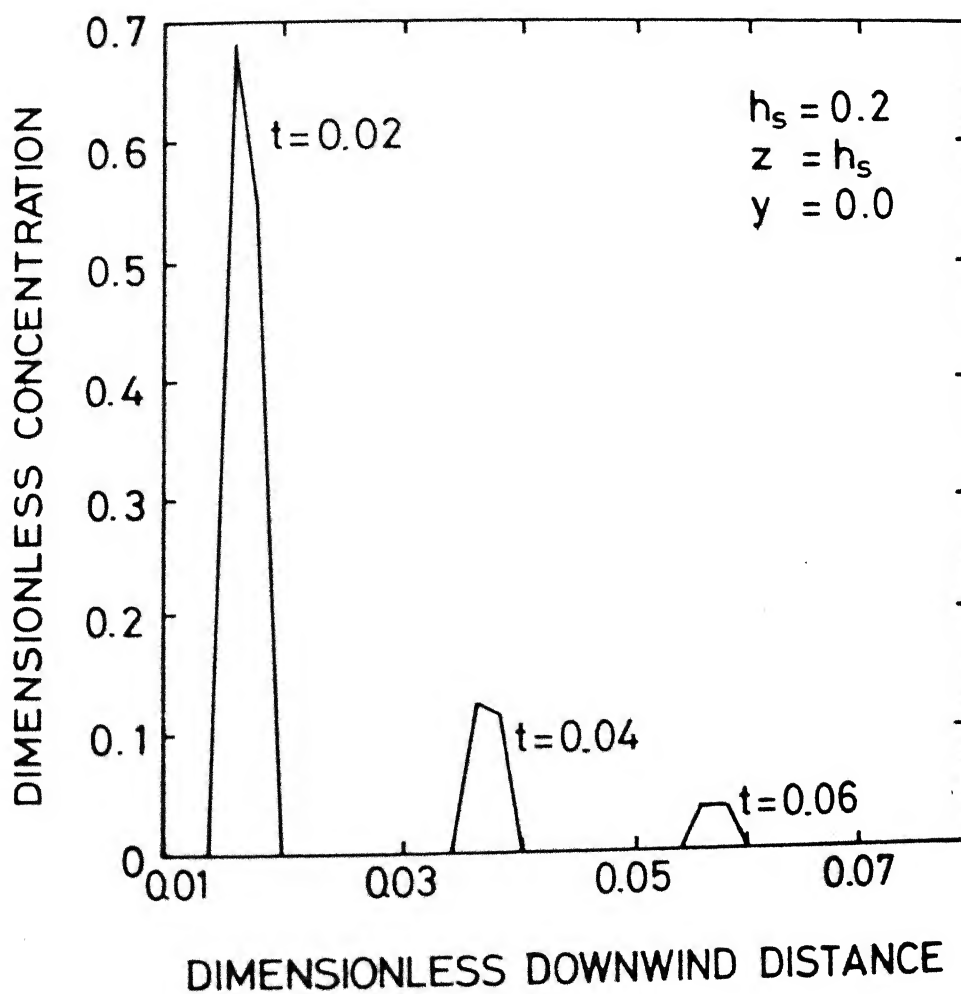


FIG. 5.3 CONCENTRATION-DISTANCE PROFILES IN RAIN DROPLET PHASE FOR INSTANTANEOUS FLUX AT THE SOURCE.

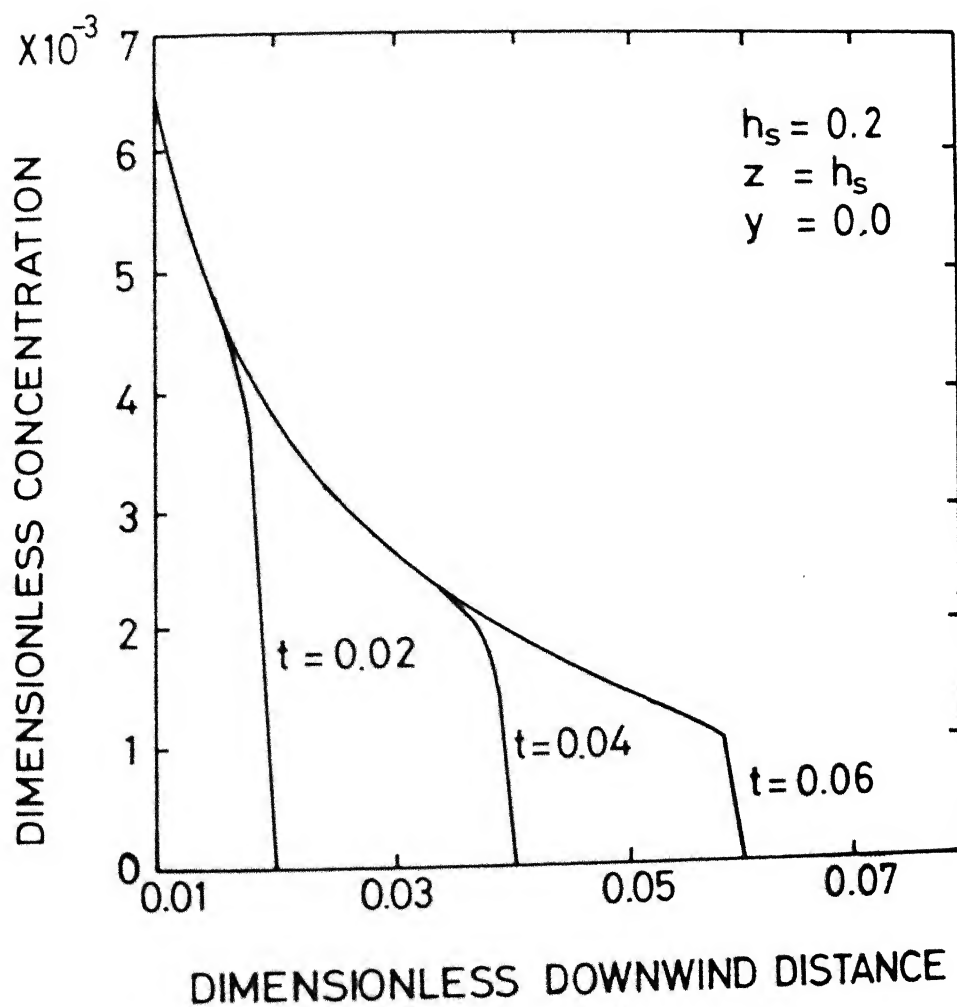


FIG. 5.4 CONCENTRATION-DISTANCE PROFILES IN RAIN DROPLET PHASE FOR CONSTANT FLUX AT THE SOURCE.

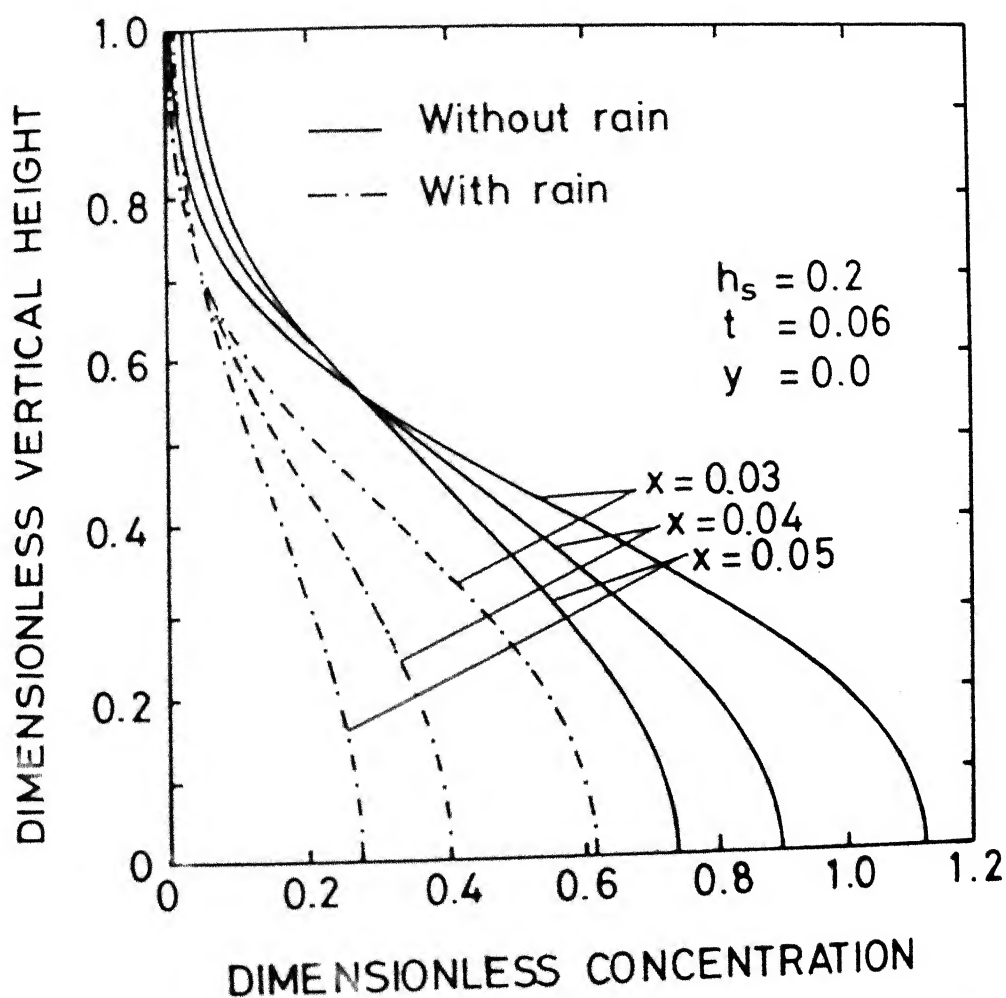


FIG.5.5 VERTICAL CONCENTRATION PROFILES IN GASEOUS PHASE FOR CONSTANT FLUX AT THE SOURCE.

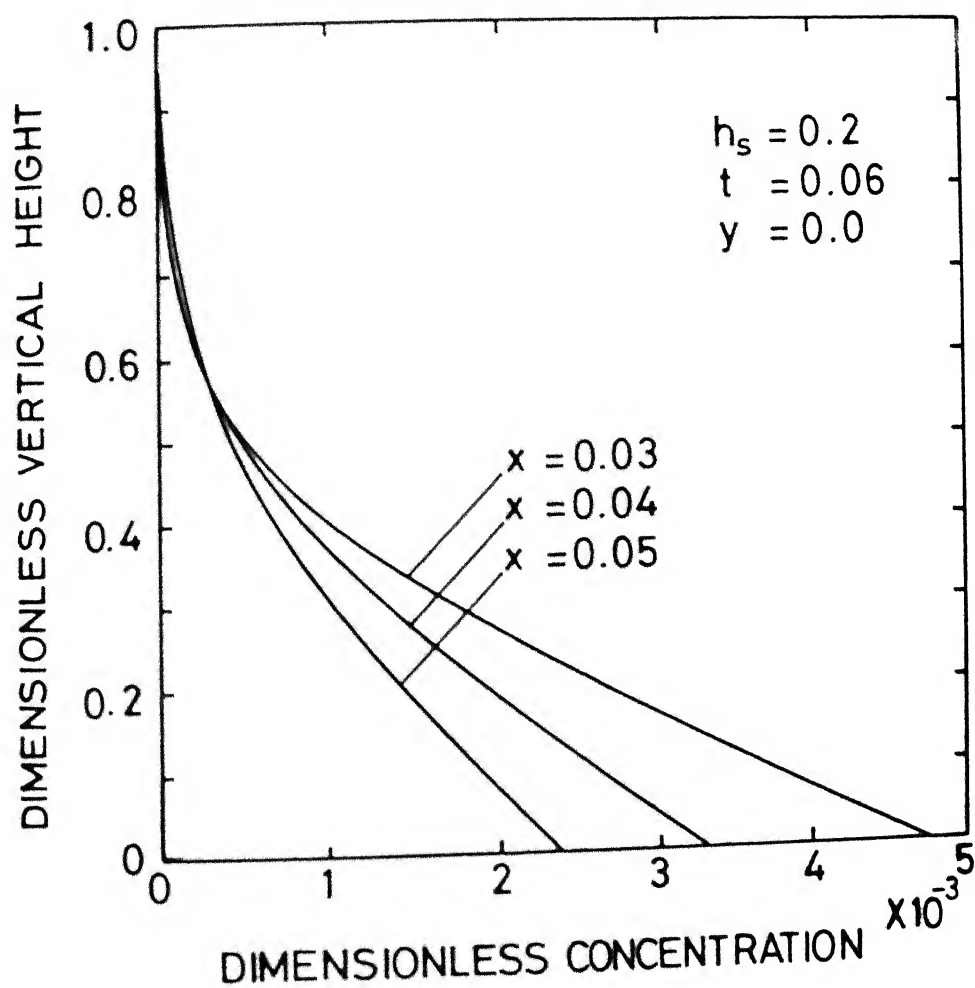


FIG.5.6 VERTICAL CONCENTRATION PROFILES IN RAIN DROPLET PHASE FOR CONSTANT FLUX AT THE SOURCE.

## CHAPTER VI

# EFFECT OF PRECIPITATION SCAVENGING ON DISPERSION OF AIR POLLUTANT IN A TWO PATCH ENVIRONMENT

### 6.0 INTRODUCTION

Since the precipitation scavenging is one of the important mechanism to remove the pollutants from the atmosphere, it has received considerable attention during the last few years as described in chapter V, [Hales(1972), Scriven and Fisher(1975a,b), Slinn(1974), Kumar(1985), Shukla *et al.*(1991a)], where we have discussed the effect of precipitation scavenging on the unsteady state dispersion of a reactive air pollutant emitted from a time dependent point source without considering patchiness in the atmosphere which arises naturally in the atmosphere with different topographical and meteorological conditions at different places.

In this chapter we, therefore, study the effect of precipitation scavenging on the unsteady state dispersion of a reactive air pollutant emitted from a time dependent point source in a two patch environment assuming that rain droplets, uniformly distributed in the second patch, absorb the pollutant and remove it by their fall on the ground. We consider that the concentration of the pollutant in both the patches is governed by the unsteady state three dimensional convective diffusion equations with different removal and other parameters. However, the concentration of the absorbed pollutant in the droplets in the second patch is

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Part of this chapter is to appear in the *Proceedings of Fifth International Conference on Precipitation Scavenging and Atmosphere-Surface Exchange Processes*, 15-19 July, 1991, Richland, Washington, U.S.A.



governed by a simplified equation which neglects diffusion term but takes into account the falling of rain droplets on the ground. To determine the concentration distributions, in the two patches i.e., without rain and with rain, these equations are solved using appropriate initial and boundary conditions, with a view to study the effect of precipitation scavenging in cleaning the environment.

As before, we consider the time dependent flux at the source to be of the forms: (i) Instantaneous, and(ii) Constant.

### 6.1 MATHEMATICAL MODEL

Consider the unsteady state dispersion of a reactive air pollutant emitted from a time dependent point source in a two patch environment. It is assumed that the point source of strength  $Q(t)$  is located in the first patch at a height  $h_s$  whereas the rain takes place in the second patch below the cloud base located at height  $z = H$ . (see Figure 6.1)

The differential equations governing the concentration distribution in both the patches are written as,

Patch I ( $0 \leq x < x_1$ ,  $0 \leq z \leq H$ )

The concentration  $C_1(x,y,z,t)$  of the pollutant in the gaseous phase in the first patch is governed by,

$$\frac{\partial C_1}{\partial t} + u_1 \frac{\partial C_1}{\partial x} = K_{y1} \frac{\partial^2 C_1}{\partial y^2} + K_{z1} \frac{\partial^2 C_1}{\partial z^2} - k_1 C_1 \quad (6.1)$$

where  $x$ ,  $y$ ,  $z$  are cartesian coordinates,  $t$  is the time,  $x$ -axis is taken along the wind direction,  $z$ -axis vertically upwards,  $u_1$  is the mean wind velocity,  $K_{y1}$  and  $K_{z1}$  are constant diffusivities in  $y$  and  $z$  directions respectively and  $k_1$  is the removal rate

coefficient of the pollutant due to some natural mechanism.

The initial and boundary conditions for equation (6.1) are,

$$C_1(x, y, z, t) = 0 \quad \text{at} \quad t = 0 \quad (6.2)$$

$$C_1(x, y, z, t) = \frac{Q(t)}{u_1} \delta(y) \delta(z - h_s) \quad \text{at} \quad x = 0 \quad (6.3)$$

$$C_1(x, y, z, t) = 0 \quad \text{as} \quad y \rightarrow \pm \infty \quad (6.4)$$

$$K_{z1} \frac{\partial C_1}{\partial z} = v_{d1} C_1 \quad \text{at} \quad z = 0 \quad (6.5)$$

$$\frac{\partial C_1}{\partial z} = 0 \quad \text{at} \quad z = H \quad (6.6)$$

where  $v_{d1}$  is the deposition velocity of the pollutant in the first patch at the ground  $z = 0$  and  $\delta(\cdot)$  is the Dirac delta function.

The following forms of time dependent flux are prescribed at the source as in the previous chapter,

(i) Flux is Instantaneous,  $Q(t) = Q_0 \delta(t)$

(ii) Flux is Constant,  $Q(t) = Q_c$

Patch II ( $x \geq x_1$ ,  $0 \leq z \leq H$ )

In this patch, where rain takes place, we assume that uniformly distributed rain droplets absorb the pollutant and remove it by their fall on the ground. The concentration of the pollutant in the gaseous phase is governed by the unsteady state three dimensional convective diffusion equation with removal and other parameters.

The concentration  $C_2(x, y, z, t)$  of the same pollutant in the second patch is governed by,

$$\frac{\partial C_2}{\partial t} + u_2 \frac{\partial C_2}{\partial x} = K_{y2} \frac{\partial^2 C_2}{\partial y^2} + K_{z2} \frac{\partial^2 C_2}{\partial z^2} - (k_2 + k_g) C_2 \quad (6.7)$$

where  $u_2$  is the mean wind velocity,  $K_{y2}$  and  $K_{z2}$  are constant diffusivities in  $y$  and  $z$  directions respectively and  $k_2$  is the natural removal rate coefficient and  $k_g$  is the depletion rate coefficient of the pollutant due to precipitation scavenging by rain.

The initial and boundary conditions for equation (6.7) are,

$$C_2(x, y, z, t) = 0 \quad \text{at} \quad t = 0 \quad (6.8)$$

$$C_2(x, y, z, t) = C_1(x, y, z, t) \quad \text{at} \quad x = x_1 \quad (6.9)$$

$$C_2(x, y, z, t) = 0 \quad \text{as} \quad y \rightarrow \pm \infty \quad (6.10)$$

$$K_{z2} \frac{\partial C_2}{\partial z} = v_{d2} C_2 \quad \text{at} \quad z = 0 \quad (6.11)$$

$$\frac{\partial C_2}{\partial z} = 0 \quad \text{at} \quad z = H \quad (6.12)$$

where  $v_{d2}$  is the deposition velocity of the pollutant in the second patch at the ground  $z = 0$ .

The concentration  $C_a(x, y, z, t)$  of the absorbed pollutant in the droplet phase is assumed to be governed by the following equation,

$$\frac{\partial C_a}{\partial t} - w \frac{\partial C_a}{\partial z} = \gamma C_2 - \eta C_a \quad (6.13)$$

with initial and boundary conditions,

$$C_a(x, y, z, t) = 0 \quad \text{at} \quad t = 0 \quad (6.14)$$

$$C_a(x, y, z, t) = 0 \quad \text{at} \quad z = H \quad (6.15)$$

where  $w$ , assumed to be constant, is the terminal velocity of rain droplets falling on the ground,  $\gamma$  ( $\leq k_g$ ) is the rate coefficient

of increase of  $C_a$  and  $\eta$  is its removal rate coefficient in the environment.

Introduce the following dimensionless quantities,

$$\bar{t} = \frac{K_{z0} t}{H^2}, \quad \bar{x} = \frac{K_{z0} x}{H^2 u_0}, \quad \bar{y} = \frac{y}{H}, \quad \bar{z} = \frac{z}{H}, \quad \bar{h}_s = \frac{h_s}{H}$$

$$\bar{u}_i = \frac{u_i}{u_0}, \quad \bar{Q}(t) = \frac{Q(t)}{Q_c}, \quad \bar{Q}_0 = \frac{Q_0 K_{z0}}{Q_c H^2}, \quad \bar{C}_i = \frac{u_0 H^2}{Q_c} C_i, \quad i = 1, 2$$

$$\bar{C}_a = \frac{u_0 H^2}{Q_c} C_a, \quad \bar{w} = \frac{H w}{K_{z0}}, \quad \bar{\gamma} = \frac{H^2 \gamma}{K_{z0}}, \quad \bar{\eta} = \frac{H^2 \eta}{K_{z0}}$$

where  $K_{z0}$  and  $u_0$  are reference diffusion coefficient and wind velocity respectively.

The equations (6.1)-(6.15) are written in dimensionless form as, (dropping bars for convenience)

Patch I ( $0 \leq x < x_1$ ,  $0 \leq z \leq 1$ )

$$\frac{\partial C_1}{\partial t} + u_1 \frac{\partial C_1}{\partial x} = \beta_1 \frac{\partial^2 C_1}{\partial y^2} + \gamma_1 \frac{\partial^2 C_1}{\partial z^2} - \alpha_1 C_1 \quad (6.16)$$

$$C_1(x, y, z, t) = 0 \quad \text{at} \quad t = 0 \quad (6.17)$$

$$C_1(x, y, z, t) = \frac{Q(t)}{u_1} \delta(y) \delta(z - h_s) \quad \text{at} \quad x = 0 \quad (6.18)$$

$$C_1(x, y, z, t) = 0 \quad \text{as} \quad y \rightarrow \pm \infty \quad (6.19)$$

$$\frac{\partial C_1}{\partial z} = N_1 C_1 \quad \text{at} \quad z = 0 \quad (6.20)$$

$$\frac{\partial C_1}{\partial z} = 0 \quad \text{at} \quad z = 1 \quad (6.21)$$

and

(i) Flux is Instantaneous,  $Q(t) = Q_0 \delta(t)$

(ii) Flux is Constant,  $Q(t) = 1$

Patch II ( $x \geq x_1$ ,  $0 \leq z \leq 1$ )

$$\frac{\partial C_2}{\partial t} + u_2 \frac{\partial C_2}{\partial x} = \beta_2 \frac{\partial^2 C_2}{\partial y^2} + \gamma_2 \frac{\partial^2 C_2}{\partial z^2} - (\alpha_2 + \alpha_g) C_2 \quad (6.22)$$

$$C_2(x, y, z, t) = 0 \quad \text{at} \quad t = 0 \quad (6.23)$$

$$C_2(x, y, z, t) = C_1(x, y, z, t) \quad \text{at} \quad x = x_1 \quad (6.24)$$

$$C_2(x, y, z, t) = 0 \quad \text{as} \quad y \rightarrow \pm \infty \quad (6.25)$$

$$\frac{\partial C_2}{\partial z} = N_2 C_2 \quad \text{at} \quad z = 0 \quad (6.26)$$

$$\frac{\partial C_2}{\partial z} = 0 \quad \text{at} \quad z = 1 \quad (6.27)$$

and

$$\frac{\partial C_a}{\partial t} - w \frac{\partial C_a}{\partial z} = \gamma C_2 - \eta C_a \quad (6.28)$$

$$C_a(x, y, z, t) = 0 \quad \text{at} \quad t = 0 \quad (6.29)$$

$$C_a(x, y, z, t) = 0 \quad \text{at} \quad z = 1 \quad (6.30)$$

where

$$\beta_i = \frac{K_{yi}}{K_{zo}}, \gamma_i = \frac{K_{zi}}{K_{zo}}, N_i = \frac{v_{di} H}{K_{zi}} \quad i = 1, 2$$

## 6.2 CONCENTRATION DISTRIBUTIONS

The system of equations (6.16)-(6.30) is solved for different forms of flux as described earlier and solutions are obtained in each case as follows,

### 6.2.1 CASE I WHEN FLUX IS INSTANTANEOUS AT THE SOURCE

$$C_1(x, y, z, t) = \frac{Q_0}{u_1} P(x, y, z) \delta\left(t - \frac{x}{u_1}\right) \quad (6.31)$$

$$C_2(x, y, z, t) = \frac{Q_0}{u_1} Q(x, y, z) \delta\left[t - \left(\frac{x_1}{u_1} + \frac{x - x_1}{u_2}\right)\right] \quad (6.32)$$

$$C_a(x, y, z, t) = \frac{Q_0 \gamma}{u_1} M(x, y, z, t) \quad (6.33)$$

where

$$P(x, y, z) = \frac{e^{-y^2/(4\frac{\beta_1}{u_1}x)}}{\sqrt{4\pi\frac{\beta_1}{u_1}x}} \sum_{n=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \gamma_1 \lambda_n^2}{u_1}\right)x\right) \frac{F_n(h_s)}{P_n} F_n(z)$$

$$Q(x, y, z) = \frac{e^{-y^2/4\beta(x)}}{\sqrt{4\pi\beta(x)}} \sum_{n=1}^{\infty} \exp\left(-\left(\frac{\alpha_2 + \alpha_g + \gamma_2 \mu_n^2}{u_2}\right)(x - x_1)\right) \frac{G_n(z)}{Q_n}$$

$$\sum_{m=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \gamma_1 \lambda_m^2}{u_1}\right)x_1\right) \frac{F_m(h_s)}{P_m} \int_0^1 F_m(z) G_n(z) dz$$

$$M(x, y, z) = \frac{e^{-y^2/4\beta(x)}}{\sqrt{4\pi\beta(x)}} \sum_{n=1}^{\infty} \exp\left(-\left(\frac{\alpha_2 + \alpha_g + \gamma_2 \mu_n^2}{u_2}\right)(x - x_1)\right) \frac{f_n(x, z, t)}{Q_n}$$

$$\sum_{m=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \gamma_1 \lambda_m^2}{u_1}\right)x_1\right) \frac{F_m(h_s)}{P_m} \int_0^1 F_m(z) G_n(z) dz$$

$$F_n(z) = \cos \lambda_n z + \frac{N_1}{\lambda_n} \sin \lambda_n z$$

$$G_n(z) = \cos \mu_n z + \frac{N_2}{\mu_n} \sin \mu_n z$$

$$P_n = \int_0^1 \left(\cos \lambda_n z + \frac{N_1}{\lambda_n} \sin \lambda_n z\right)^2 dz$$

$$Q_n = \int_0^1 \left(\cos \mu_n z + \frac{N_2}{\mu_n} \sin \mu_n z\right)^2 dz$$

Here  $\lambda_n$  and  $\mu_n$  are the roots of the following transcendental equations respectively,

$$\lambda_n \tan \lambda_n = N_1$$

$$\mu_n \tan \mu_n = N_2, \quad n = 1, 2, 3, \dots$$

$$\begin{aligned} f_n(x, z, t) = & -f_{n1}(x, z, t) \left( \cos \mu_n + \frac{N_2}{\mu_n} \sin \mu_n \right) \\ & + f_{n2}(x, z, t) \left( -N_2 \cos \mu_n + \mu_n \sin \mu_n \right) \\ & + f_{n3}(x, z, t) \left( \cos \mu_n z + \frac{N_2}{\mu_n} \sin \mu_n z \right) \\ & + f_{n4}(x, z, t) \left( N_2 \cos \mu_n z - \mu_n \sin \mu_n z \right) \end{aligned}$$

$$f_{n1}(x, z, t) = \text{ex11} \cos(\arg 1) H \left( t - \left( \frac{x_1}{u_1} + \frac{x-x_1}{u_2} + \frac{1-z}{w} \right) \right) H \left( t - \frac{1-z}{w} \right)$$

$$f_{n2}(x, z, t) = \frac{\text{ex11}}{\mu_n} \sin(\arg 1) H \left( t - \left( \frac{x_1}{u_1} + \frac{x-x_1}{u_2} + \frac{1-z}{w} \right) \right) H \left( t - \frac{1-z}{w} \right)$$

$$f_{n3}(x, z, t) = \text{ex11} \cos(\arg 2) H \left( t - \left( \frac{x_1}{u_1} + \frac{x-x_1}{u_2} \right) \right)$$

$$f_{n4}(x, z, t) = \frac{\text{ex11}}{\mu_n} \sin(\arg 2) H \left( t - \left( \frac{x_1}{u_1} + \frac{x-x_1}{u_2} \right) \right)$$

$$\arg 1 = \mu_n w \left( t - \left( \frac{x_1}{u_1} + \frac{x-x_1}{u_2} + \frac{1-z}{w} \right) \right)$$

$$\arg 2 = \mu_n w \left( t - \left( \frac{x_1}{u_1} + \frac{x-x_1}{u_2} \right) \right)$$

$$\text{ex11} = \exp \left\{ -\eta \left( t - \left( \frac{x_1}{u_1} + \frac{x-x_1}{u_2} \right) \right) \right\}$$

$$\beta(x) = \frac{\beta_1}{u_1} x_1 + \frac{\beta_2}{u_2} (x - x_1)$$

### 6.2.2 CASE II WHEN FLUX IS CONSTANT AT THE SOURCE

$$C_1(x, y, z, t) = \frac{1}{u_1} P(x, y, z) H\left(t - \frac{x}{u_1}\right) \quad (6.34)$$

$$C_2(x, y, z, t) = \frac{1}{u_1} Q(x, y, z) H\left(t - \left(\frac{x_1}{u_1} + \frac{x-x_1}{u_2}\right)\right) \quad (6.35)$$

$$C_a(x, y, z, t) = \frac{\gamma}{u_1} N(x, y, z, t) \quad (6.36)$$

where

$$N(x, y, z, t) = \frac{e^{-y^2/4\beta(x)}}{\sqrt{4\pi\beta(x)}} \sum_{n=1}^{\infty} \exp\left(-\left(\frac{\alpha_2 + \alpha_g + \gamma_2 \mu_n^2}{u_2}\right)(x - x_1)\right) \frac{g_n(x, z, t)}{Q_n} \\ \sum_{m=1}^{\infty} \exp\left(-\left(\frac{\alpha_1 + \gamma_1 \lambda_m^2}{u_1}\right)x_1\right) \frac{F_m(h_s)}{P_m} \int_0^1 F_m(z) G_n(z) dz$$

$$g_n(x, z, t) = -g_{n1}(x, z, t) \left(\cos \mu_n + \frac{N_2}{\mu_n} \sin \mu_n\right) \\ + g_{n2}(x, z, t) \left(-N_2 \cos \mu_n + \mu_n \sin \mu_n\right) \\ + g_{n3}(x, z, t) \left(\cos \mu_n z + \frac{N_2}{\mu_n} \sin \mu_n z\right) \\ + g_{n4}(x, z, t) \left(N_2 \cos \mu_n z - \mu_n \sin \mu_n z\right)$$

$$g_{n1}(x, z, t) = \left[ \frac{\exp\{[-\eta \cos(\arg 1) + \mu_n w \sin(\arg 1)] + \eta e^{-\eta(1-z)/w}\}}{\eta^2 + \mu_n^2 w^2} \right] \\ \times H\left(t - \left(\frac{x_1}{u_1} + \frac{x-x_1}{u_2} + \frac{1-z}{w}\right)\right) H\left(t - \frac{1-z}{w}\right)$$

$$g_{n2}(x, z, t) = \left[ \frac{\exp\{[-\eta \sin(\arg 1) - \mu_n w \cos(\arg 1)] + \mu_n w e^{-\eta(1-z)/w}\}}{\mu_n(\eta^2 + \mu_n^2 w^2)} \right] \\ \times H\left(t - \left(\frac{x_1}{u_1} + \frac{x-x_1}{u_2} + \frac{1-z}{w}\right)\right) H\left(t - \frac{1-z}{w}\right)$$



$$g_{n3}(x,z,t) = \left[ \frac{\exp\{[-\eta \cos(\arg 2) + \mu_n w \sin(\arg 2)] + \eta\}}{\eta^2 + \mu_n^2 w^2} \right] H\left(t - \left(\frac{x_1}{u_1} + \frac{x-x_1}{u_2}\right)\right)$$

$$g_{n4}(x,z,t) = \left[ \frac{\exp\{[-\eta \sin(\arg 2) - \mu_n w \cos(\arg 2)] + \mu_n w\}}{\mu_n(\eta^2 + \mu_n^2 w^2)} \right] H\left(t - \left(\frac{x_1}{u_1} + \frac{x-x_1}{u_2}\right)\right)$$

### 6.3 DISCUSSION AND RESULTS

To see the effect of removal parameters, the expressions for concentration of pollutant in both the patches and that of the absorbed pollutant in the droplets have been computed and shown in Figures 6.2-6.9. The parameters values used in the computation are  $Q_0 = 1.0$ ,  $\alpha_1 = 2.00$ ,  $\alpha_2 = 2.0$ ,  $\alpha_g = 20.0$ ,  $\beta_1 = \beta_2 = 10.0$ ,  $u_1 = u_2 = 1.0$ ,  $\gamma_1 = \gamma_2 = 1.0$ ,  $N_1 = 2.0$ ,  $N_2 = 0.04$ ,  $w = 1000$ ,  $h_s = 0.2$ ,  $\gamma = 18.0$ ,  $\eta = 0.01$ ,  $x_1 = 0.04$ ,  $y = 0.0$ ,  $\epsilon = 0.005$ .

When flux is instantaneous at the source, the central line concentrations of the pollutant in gaseous phase with and without rain with downwind distance are shown in Figure 6.2 for different values of  $t$ . It is observed that the concentrations with and without precipitation scavenging decrease as time increases but this decrease is considerably enhanced due to precipitation scavenging.

The central line concentrations of the pollutant in gaseous phase versus downwind distance with and without rain for constant source are shown in Figure 6.3 for different values of  $t$ . It is noted that the concentrations of pollutant with and without rain increase as time increases and reach their respective steady state values as  $t \rightarrow \infty$ . It is also concluded that the concentration of the pollutant reduced considerably due to precipitation in the second patch i.e.,  $x > x_1 = 0.04$ .

The concentration of the absorbed pollutant  $C_a$  in rain droplets along the center line  $(0,0,h_s)$  with downwind distance for both instantaneous and constant source is shown in Figure 6.4 and 6.5 for different values of  $t$ . It is observed that this concentration decreases as time increases for instantaneous source and increases with time for constant source and reaches its steady state value as  $t \rightarrow \infty$ .

In Figure 6.6 the concentrations of the pollutant in gaseous phase with and without rain for constant source are plotted with vertical height at a particular time  $t = 0.10$  for three values of  $x = 0.07, 0.08, 0.09$ . The concentration of the pollutant decreases as  $x$  increases at a time  $t > x$ . It is also seen that the concentration of the pollutant decreases due to precipitation scavenging by rain.

In Figure 6.7 the variation of concentration of the absorbed pollutant in rain droplet phase with vertical height is shown for different values of  $x$  at  $t = 0.10$ . It is noted that this concentration increases with decrease in height but decreases as  $x$  increases for  $t > x$ .

When  $x_1 = 0.001$ , i.e. when the second patch where rain takes place is closer to the source, the vertical concentration profiles of the pollutant in gaseous phase with and without rain for constant source are shown in Figure 6.8 for different values of  $x = 0.03, 0.04, 0.05$ . It is found that this figure is approximately same to Figures 5.5 of the preceding chapter without patchiness in the atmosphere showing the importance of the location of the second patch from the source where precipitation is taking place. Similar result is also valid for absorbed pollutant in the droplet

phase for constant source. (See Figures 6.9 and 5.6).

Finally, from the above analysis and the results in chapter V, it may be concluded that precipitation scavenging is a very important mechanism for the removal of the pollutant from the atmosphere at a given receptor point located in the second patch. However, the rate of reduction depends upon the location of the patch and prevailing meteorological conditions. It may also be noted that the reduction in pollutant concentration is larger at the receptor when precipitation patch is closer to the source.

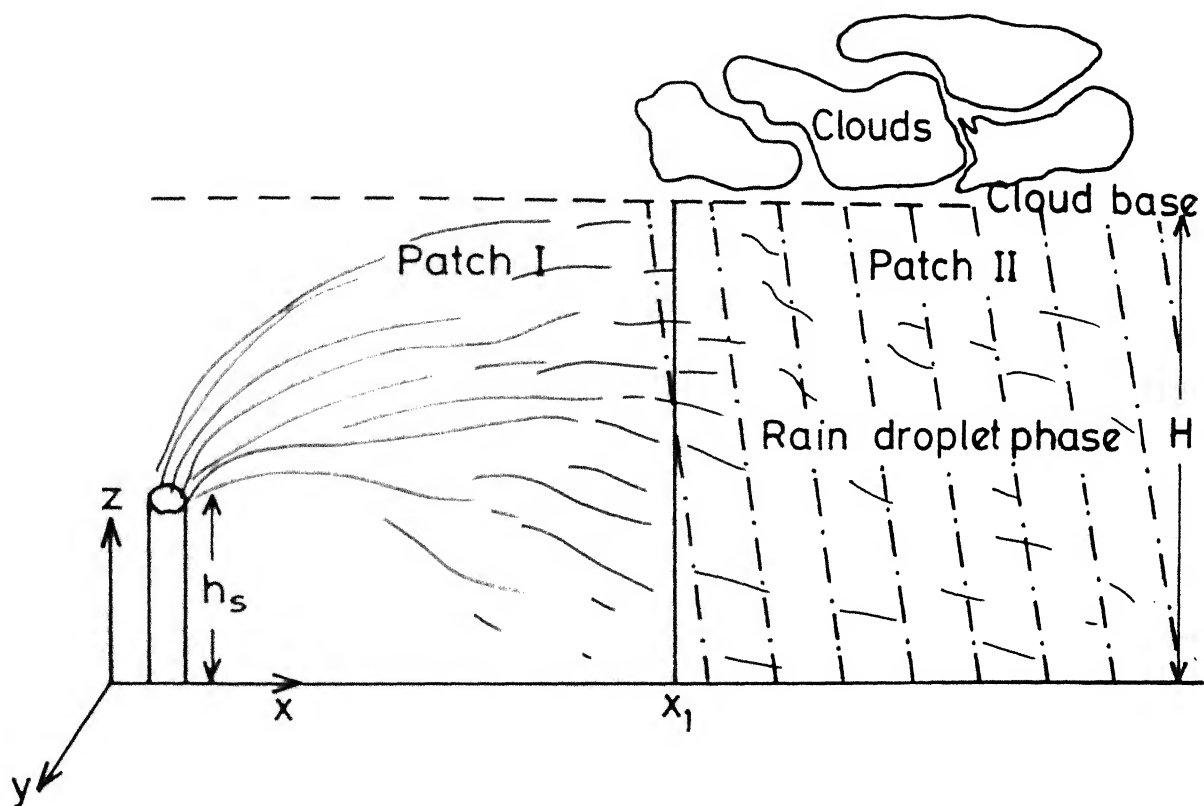


FIG.6.1 DISPERSION OF AIR POLLUTANT AND ITS REMOVAL BY PRECIPITATION SCAVENGING IN THE SECOND PATCH.

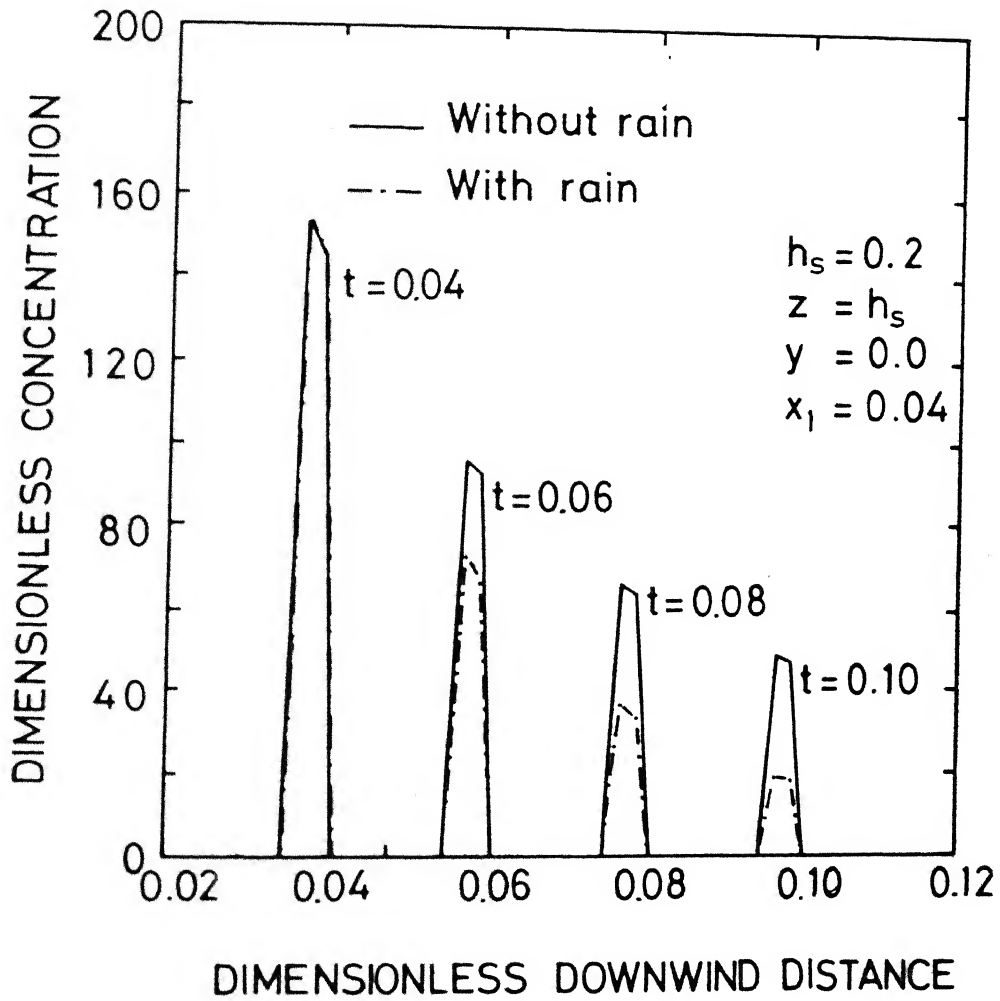


FIG. 6.2 CONCENTRATION-DISTANCE PROFILES IN GASEOUS PHASE FOR INSTANTANEOUS FLUX AT THE SOURCE.

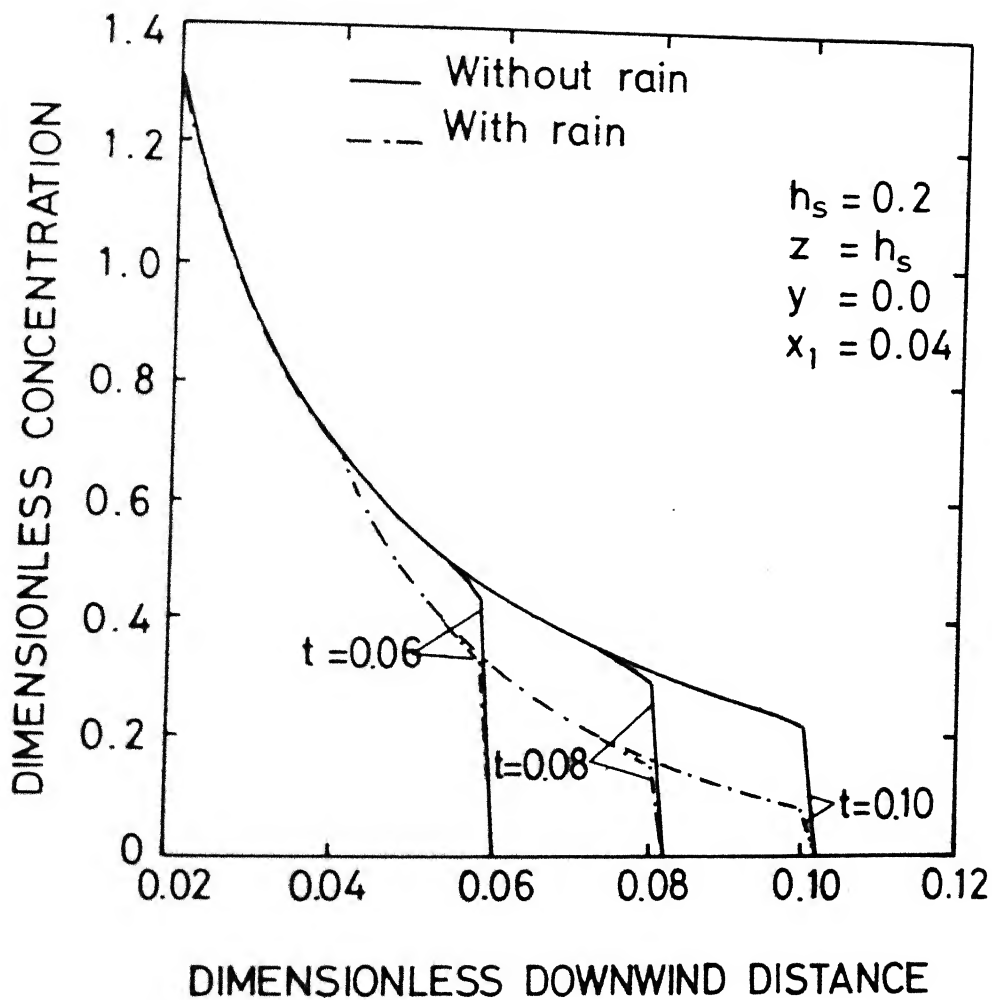


FIG.6.3 CONCENTRATION-DISTANCE PROFILES IN GASEOUS PHASE FOR CONSTANT FLUX AT THE SOURCE.

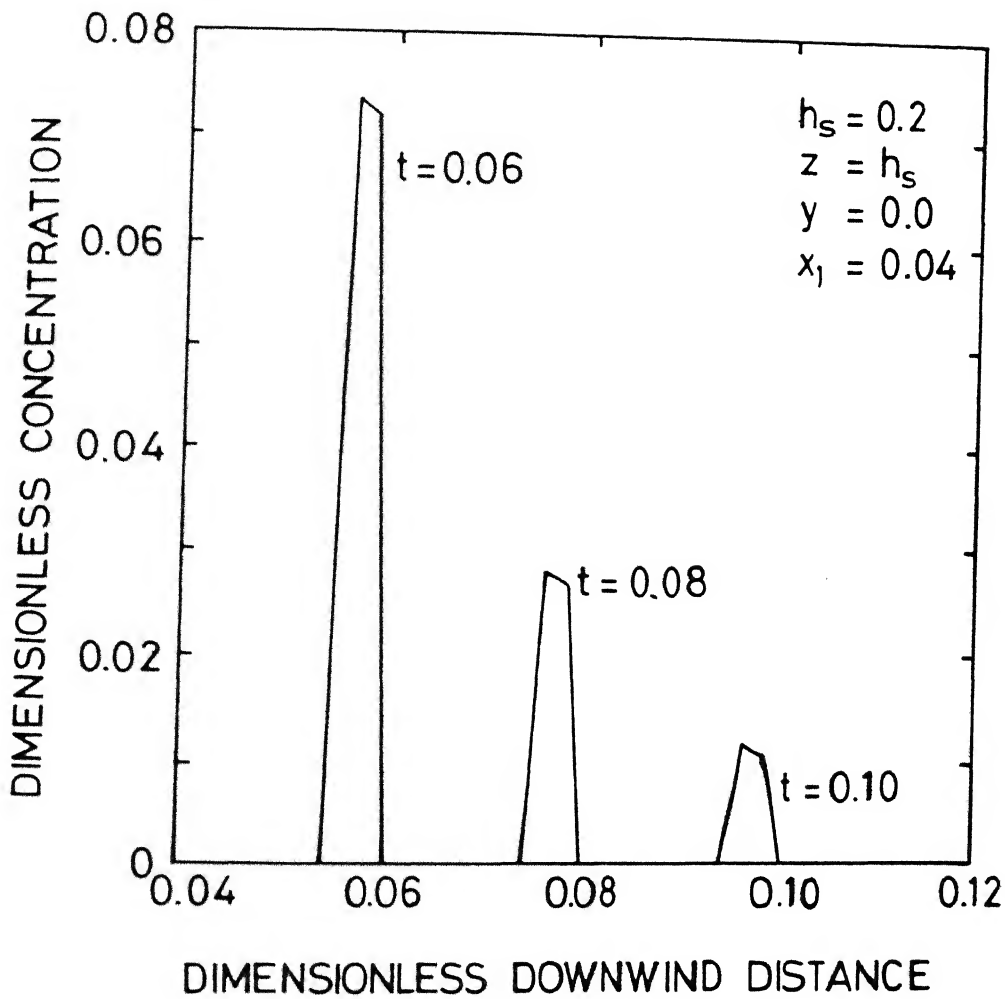


FIG.6.4 CONCENTRATION-DISTANCE PROFILES IN RAIN DROPLET PHASE FOR INSTANTANEOUS FLUX AT THE SOURCE.

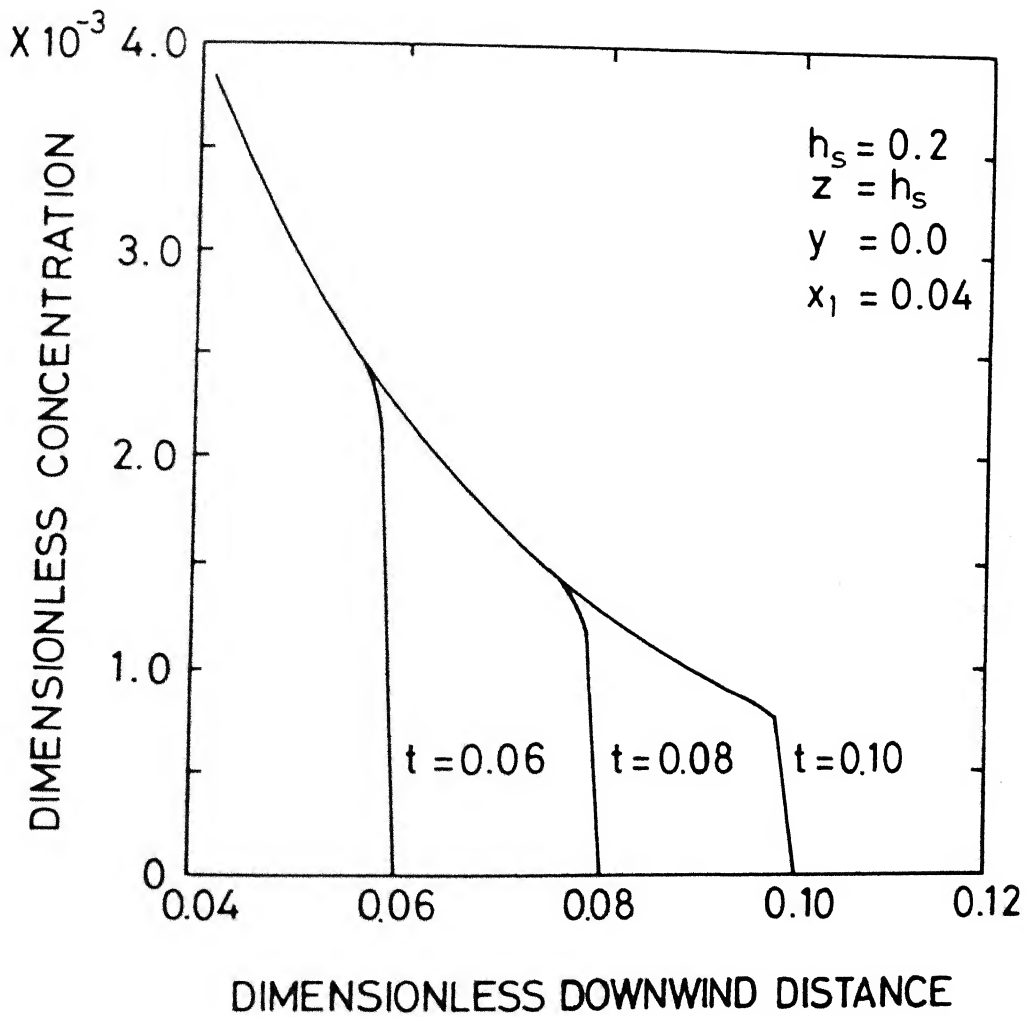


FIG.6.5 CONCENTRATION-DISTANCE PROFILES IN RAIN DROPLET PHASE FOR CONSTANT FLUX AT THE SOURCE.



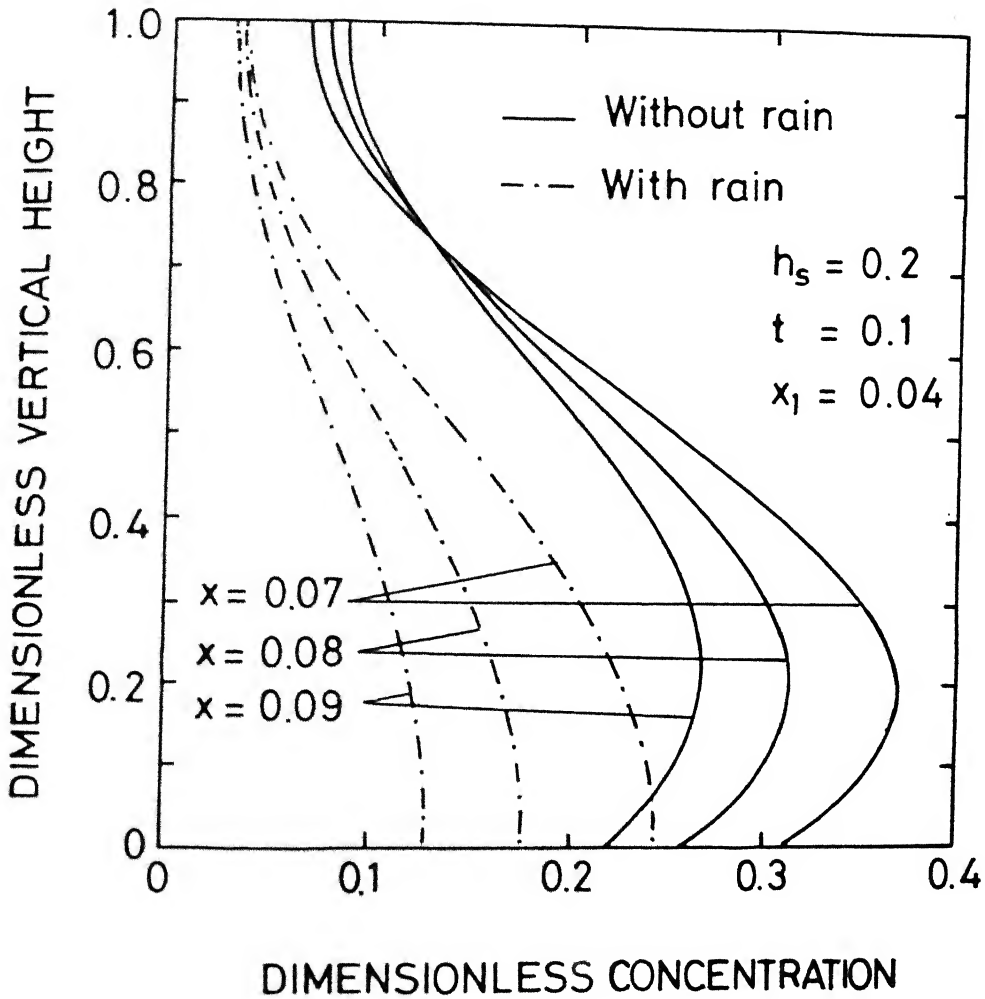


FIG. 6.6 VERTICAL CONCENTRATION PROFILES IN GASEOUS PHASE FOR CONSTANT FLUX AT THE SOURCE.

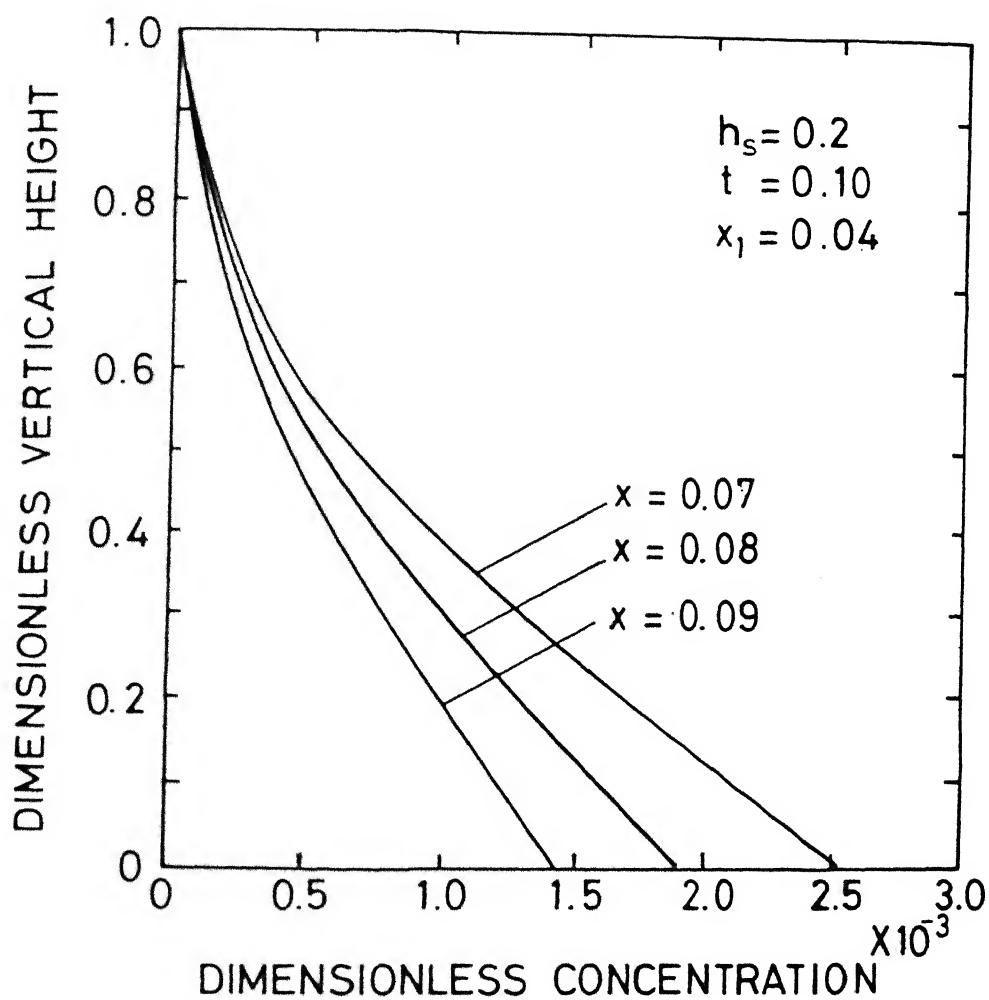


FIG.6.7 VERTICAL CONCENTRATION PROFILES IN RAIN DROPLET PHASE FOR CONSTANT FLUX AT THE SOURCE.

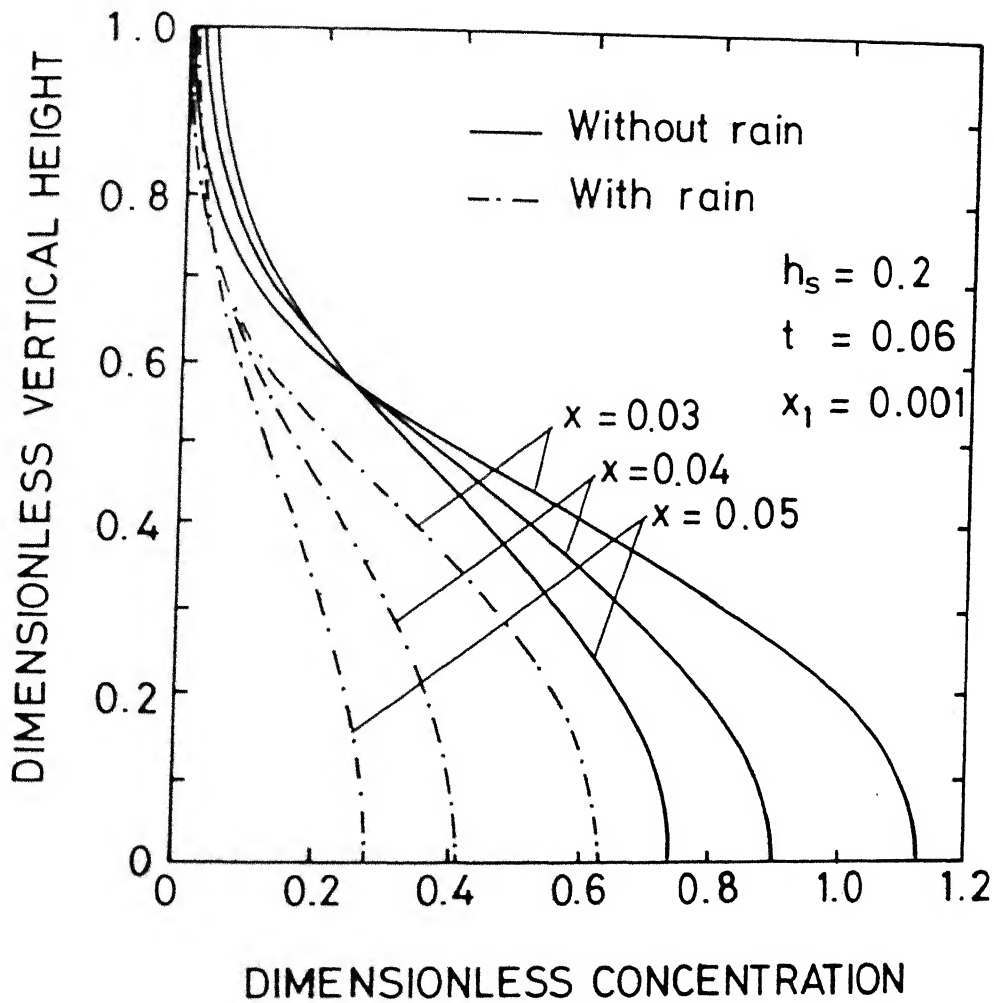


FIG.6.8 VERTICAL CONCENTRATION PROFILES IN GASEOUS PHASE FOR CONSTANT FLUX AT THE SOURCE.

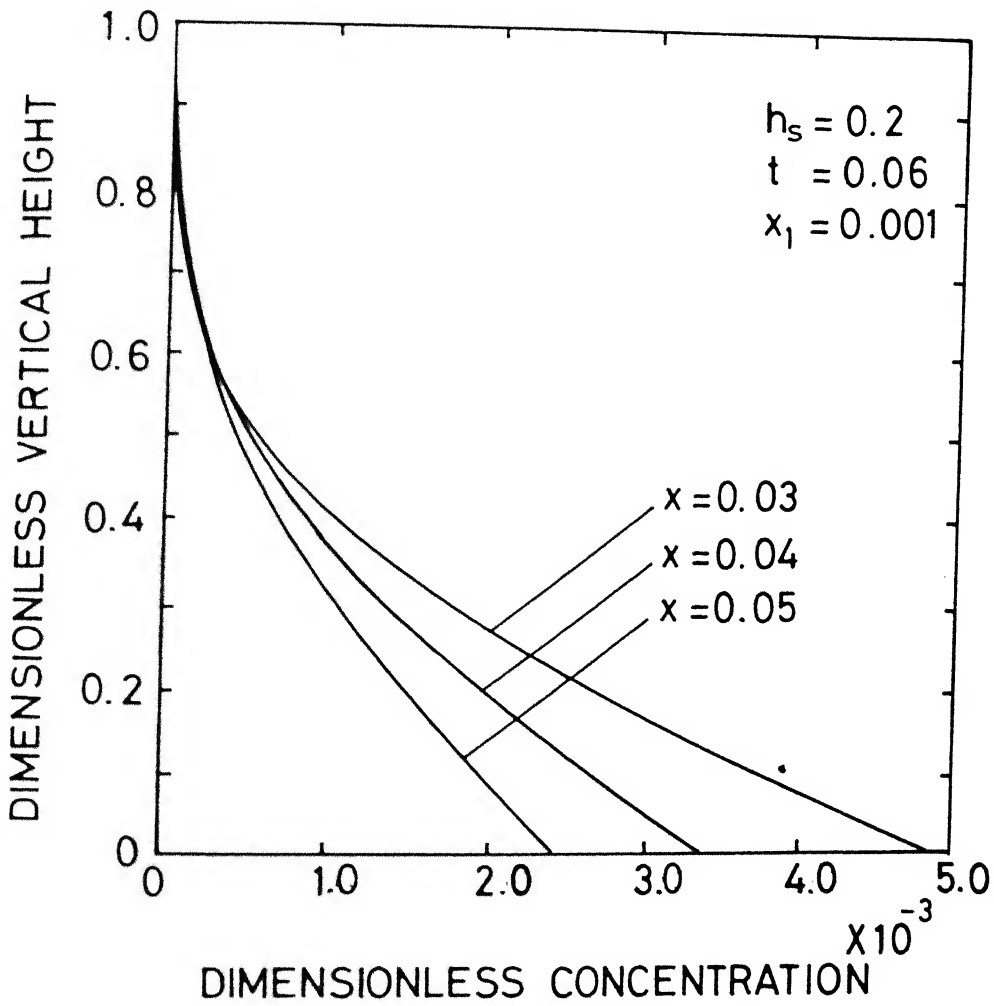


FIG.6.9 VERTICAL CONCENTRATION PROFILES IN RAIN DROPLET PHASE FOR CONSTANT FLUX AT THE SOURCE.

## CHAPTER VII

# AN ECOLOGICAL TYPE NONLINEAR PRECIPITATION MODEL FOR REMOVAL MECHANISM OF AIR POLLUTANT FORMING SECONDARY SPECIES IN THE ATMOSPHERE

### 7.0 INTRODUCTION

In the last two chapters we have proposed linear mathematical models using unsteady state three dimensional convective diffusion equation to study the effect of precipitation scavenging due to rain, on the dispersion of air pollutant from a time dependent point source. Linear models related to precipitation scavenging due to rain, fog or snow and similar situations have also been studied by Hales(1972), Slinn(1974), Fisher(1982), Shukla *et al.*(1982), Kumar(1985), Pandis and Seinfeld(1990), etc. However, it may be pointed out that in real situations during precipitation, the number density of rain, fog or snow droplets changes as the intensity of precipitation increases and this change in number density affects the interaction process and should, therefore, be taken into account in the model. The removal term, in general, due to precipitation is not only proportional to the concentration of the absorbed pollutant but is also proportional to the number density of rain droplets in the atmosphere making the phenomenon nonlinear.

Keeping in view the above, in this chapter a nonlinear ecological type precipitation model for removal mechanism of both primary and secondary pollutants is proposed by taking into account the interaction of droplet phase with the pollutant phase.

(iv) combined phase of both the pollutants absorbed in droplets.

Let  $C_r(t)$  be the number density of droplets of radius  $r$  in the droplet phase,  $C(t)$  be the concentration of the primary pollutant,  $C_p(t)$  be the concentration of the secondary pollutant and  $C_a(t)$  be the concentration of the absorbed pollutant in the droplet phase.

We now proceed to formulate the nonlinear model governing the evolution of these phases using the concepts of ecology related to growth rate, death rate and interaction process, Maynard Smith(1974), Kormondy(1986). The ideas presented here are similar to as used by Freedman and Shukla (1991) in another context. [See also Shukla *et al.*(1991c)].

In the monsoon season it is generally observed that, during precipitation, rain starts with less intensity and later it becomes more intense and continues so for days. In such a case the number density of droplets increases as time increases. Similar situation arises when snow falls on the ground. Also in the case of foggy environment the number density of fog droplets increases from some smaller value to a higher value when fog becomes more dense. Further, the growth rate of droplet phase may also change because of deposition of droplets on the ground or on vegetative canopies due to gravity, and this rate may be proportional to the number density of droplets as well as to the concentration of pollutants in the droplet phase (i.e.,  $\nu C_r C_a$ )

Under these conditions and assuming the continuity of the process, the differential equations governing the number density  $C_r(t)$  may be written, using ecological, type ideas, as follows,

(Maynard Smith, 1974)

$$\frac{dC_r}{dt} = q - r(C_a)C_r \quad (7.1)$$

where  $r(C_a) = r_0 + \nu C_a$ , and thus  $r(0) = r_0 > 0$ ,  $r'(C_a) = \nu > 0$  and  $q$  is the rate of increase of droplets in the atmosphere assumed to be constant. It may be pointed out here that in real situations this rate is time dependent and may be periodic but in this analysis  $q$  may be considered as the mean of this periodic growth rate.

To write the equations for  $C(t)$ ,  $C_p(t)$ , and  $C_a(t)$  it is assumed that the pollutant is emitted in the atmosphere at a rate  $Q(t)$ , with natural depletion rate  $\delta_0 C$ , and converted to secondary pollutant with a rate  $\lambda C$ . Thus, the rate of increase of secondary pollutant is  $\lambda C$  which may also get depleted with a rate  $\delta_1 C_p$ . The main mechanism, however, for removing pollutants (both primary and secondary) from the atmosphere is through the droplets falling on the ground and this removal rate is considered to be proportional to the number density of droplets as well as the concentration  $C_a$  in the droplet phase (i.e.,  $\nu C_r C_a$ ). Further, it is assumed that both primary and secondary pollutants are absorbed by the droplet phase in direct proportion to the concentration of the respective pollutants and the number density of droplets (i.e.,  $\alpha C C_r$  and  $\alpha_1 C_p C_r$  respectively). We also assume that the absorbed pollutant with concentration  $C_a$  in the droplet phase may be removed from the total environment directly with rate  $\delta_a C_a$  and some of it may reenter (i.e.,  $\theta \delta_a C_a$  and  $\theta_1 \delta_a C_a$ ) the atmosphere to increase the growth rate of primary and secondary pollutants if the process is reversible.

With these considerations the differential equations for  $C(t)$ ,  $C_p(t)$  and  $C_a(t)$  are written as,

$$\frac{dC}{dt} = -(\delta_0 + \lambda)C - \alpha C C_r + \theta \delta_a C_a + Q(t) \quad (7.2)$$

$$\frac{dC_p}{dt} = -\delta_1 C_p + \lambda C - \alpha_1 C_p C_r + \theta_1 \delta_a C_a \quad (7.3)$$

$$\frac{dC_a}{dt} = -\delta_a C_a + \alpha C C_r + \alpha_1 C_p C_r - \nu_a C_r C_a \quad (7.4)$$

for  $C_r(0) \geq 0$ ,  $C(0) \geq 0$ ,  $C_a(0) \geq k C_r(0)$ ,  $C_p(0) \geq 0$ , where

$\delta_0$  is the natural depletion rate coefficient of the primary pollutant in the atmosphere,

$\delta_1$  is the natural depletion rate coefficient of the secondary pollutant in the atmosphere,

$\delta_a$  is the natural depletion rate coefficient of the absorbed pollutant in the atmosphere,

$\lambda$  is the conversion rate coefficient of primary pollutant to secondary pollutant in the atmosphere,

$\alpha, \alpha_1$  are the reaction rate coefficients of primary and secondary pollutants in droplets respectively,

$\nu$  ( $\geq \nu_a$ ) is the removal rate coefficient of droplets from the atmosphere,

$\nu_a$  is the removal rate coefficient of the absorbed pollutant in droplets from the atmosphere,

$k \geq 0$  is a constant determining the initial pollutant concentration in droplet phase at  $t = 0$ , (which is naturally dependent on  $C_r(0)$  and note that for  $C_a(0) = 0$ ,  $k$  has to be zero),

$0 \leq \theta, \theta_1 \leq 1$  are the reversible rate coefficients.



We now analyze the model (7.1), (7.2), (7.3), (7.4) for  $Q(t) \equiv 0$  and  $Q(t) \equiv Q$  (constant) by using stability theory, (Lasalle and Lefschetz, 1961). The case  $Q(t) \equiv 0$  corresponds to the situation when the pollutant is emitted in the atmosphere by an instantaneous source. However, the case  $Q(t) \equiv Q$  represents the emission of pollutant in the atmosphere with a constant rate, for example, by stacks emitting continuously.

## 7.2 ANALYSIS OF THE MODEL

The analysis of the above model will be presented in two parts. We will first analyze the model assuming that there is no secondary pollutant in the atmosphere and later with the formation of secondary pollutant as well.

### 7.2a ANALYSIS WITHOUT SECONDARY POLLUTANT

In this case, in the absence of secondary pollutant, the equations (7.2), (7.3), and (7.4) reduce to the following form,

$$\frac{dC}{dt} = -\delta_0 C - \alpha C C_r + \theta \delta_a C_a + Q(t) \quad (7.5)$$

$$\frac{dC_a}{dt} = -\delta_a C_a + \alpha C C_r - \nu_a C_r C_a \quad (7.6)$$

$$C(0) \geq 0, \quad C_a(0) \geq k C_r(0)$$

We now analyze the model (7.1), (7.5), (7.6) for  $Q(t) \equiv 0$  and  $Q(t) \equiv Q$  (constant).

#### 7.2.1 CASE I $Q(t) \equiv 0$ (Instantaneous Source)

In this case our model has only one non-negative equilibria in the  $C_r$ - $C$ - $C_a$  space, namely,  $E_0(\frac{Q}{r_0}, 0, 0)$ . To determine the local stability of the equilibria, we compute the corresponding variational matrix  $M_0$  as follows,

$$M_0 = \begin{bmatrix} -r_0 & 0 & -\nu \frac{q}{r_0} \\ 0 & -(\delta_0 + \alpha \frac{q}{r_0}) & \theta \delta_a \\ 0 & \alpha \frac{q}{r_0} & -(\delta_a + \nu_a \frac{q}{r_0}) \end{bmatrix}$$

Using Routh Hurwitz theorem, from the above it is clear that  $E_0(\frac{q}{r_0}, 0, 0)$  is locally asymptotically stable in  $C_r$ - $C$ - $C_a$  plane. However, we can say much more about  $E_0$  in the form of the following theorem,

**THEOREM 7.2.1** If  $C_r(0) > 0$ , then  $E_0$  is globally asymptotically stable with respect to the non-negative octant.

**PROOF :** First we note

$$\begin{aligned} \frac{dC_r}{dt} &= \dot{C}_r = q - r(C_a)C_r \\ &\leq q - r_0 C_r \end{aligned}$$

$$\text{Hence } \lim_{t \rightarrow \infty} C_r(t) \leq \frac{q}{r_0}$$

Now consider

$$\begin{aligned} \dot{C} + \dot{C}_a &= -\left( \delta_0 C + \delta_a C_a (1 - \theta) + \nu_a C_r C_a \right) \\ &\leq -\left( \delta_0 C + \delta_a C_a (1 - \theta) \right) \\ &\leq -\delta_m (C + C_a) \end{aligned}$$

$$\text{where } \delta_m = \min(\delta_0, \delta_a(1 - \theta))$$

Therefore,  $C(t) + C_a(t) \leq (C(0) + C_a(0)) e^{-\delta_m t}$ , and hence the system is dissipative. From the above it follows that

$$\lim_{t \rightarrow \infty} C(t) = \lim_{t \rightarrow \infty} C_a(t) = 0. \text{ Hence in the limit } C_r(t) \text{ is given by}$$

the solution of  $\dot{C}_r(t) = q - r_0 C_r$ . Since  $C_r(0) > 0$ , the theorem

follows.

This theorem implies that if the pollutant is emitted in the atmosphere by an instantaneous source ( $C_r(0) > 0$ ), all the pollutant would be removed from the atmosphere by the precipitation scavenging with the number density of droplets remaining at its equilibrium.

### 7.2.2 CASE II $Q(t) \equiv Q > 0$ (Constant Source)

In this case our model has one non-negative equilibria  $\tilde{E}(\tilde{C}_r, \tilde{C}, \tilde{C}_a)$ ,

To prove that  $\tilde{E}$  exist, we show that the system of algebraic equations,

$$q - r(\tilde{C}_a)\tilde{C}_r = 0 \quad (7.7)$$

$$-\delta_0\tilde{C} - \alpha\tilde{C}\tilde{C}_r + \theta\delta_a\tilde{C}_a + Q = 0 \quad (7.8)$$

$$-\delta_a\tilde{C}_a + \alpha\tilde{C}\tilde{C}_r - \nu_a\tilde{C}_r\tilde{C}_a = 0 \quad (7.9)$$

has a positive solution.

$$\text{Equation (7.7) gives } \tilde{C}_r = \frac{q}{r(\tilde{C}_a)}, \quad (7.10)$$

substituting  $\tilde{C}_r$  in equations (7.8) and (7.9), we get

$$\tilde{C} = \frac{Q + \theta\delta_a\tilde{C}_a}{\delta_0 + \frac{\alpha q}{r(\tilde{C}_a)}} \quad (7.11)$$

$$\tilde{C} = \frac{\tilde{C}_a \left( \delta_a r(\tilde{C}_a) + q\nu_a \right)}{\alpha q} \quad (7.12)$$

We note from equation (7.11) that  $\tilde{C} \rightarrow \frac{Q r_0}{\alpha q + \delta_0 r_0} = \tilde{C}_1$  (say)  $> 0$

as  $\tilde{C}_a \rightarrow 0$ , and  $\tilde{C} \rightarrow \infty$  as  $\tilde{C}_a \rightarrow \infty$  i.e.,  $\tilde{C}$  is an increasing function of  $\tilde{C}_a$ .

Further from equation (7.12),  $\tilde{C} \rightarrow 0$  as  $\tilde{C}_a \rightarrow 0$ , and  $\tilde{C}$  is also an increasing function of  $\tilde{C}_a$ . Hence two isoclines (7.11) and (7.12) would intersect as shown in Figure 7.1, and give positive equilibrium, provided the line segment  $P_2P_3 < P_1P_3$ , where coordinate of  $P_3$  is  $(Q/\delta_m, 0)$ . This condition can be written from equation (7.11) and (7.12) as,

$$\frac{(\delta_m + \theta\delta_a)(r_0\delta_m + \nu Q)}{\{\delta_m(r_0\delta_0 + \alpha q) + \delta_0\nu Q\}} < \frac{\{\delta_a(r_0\delta_m + \nu Q) + q\nu_a\delta_m\}}{\alpha q\delta_m}$$

where  $\delta_m = \min\{\delta_0, \delta_a(1 - \theta)\}$ , see lemma 7.2.3.

From Figure 7.1 it is noted that as  $\nu_a$  increases the equilibrium values  $\tilde{C}$  and  $\tilde{C}_a$  both decrease and even may tend to zero if  $\nu_a$  is very large.

Now the variational matrix corresponding to  $\tilde{E}$  is given by  $\tilde{M}$  as follows,

$$\tilde{M} = \begin{bmatrix} -r(\tilde{C}_a) & 0 & -\nu\tilde{C}_r \\ -\alpha\tilde{C} & -(\delta_0 + \alpha\tilde{C}_r) & \theta\delta_a \\ \alpha\tilde{C} - \nu_a\tilde{C}_a & \alpha\tilde{C}_r & -(\delta_a + \nu_a\tilde{C}_r) \end{bmatrix}$$

For  $\tilde{E}$  we now find a sufficient condition for this equilibrium to be locally asymptotically stable in the form of the following theorem,

**THEOREM 7.2.2** Let the following inequalities hold,

$$2\alpha\tilde{C} < r_0 + (\nu_a + \nu)\tilde{C}_a \tag{7.13}$$

$$(\nu - \nu_a)\tilde{C}_r < \delta_a(1 - \theta)$$

then  $\tilde{E}$  is locally asymptotically stable.

PROOF : If inequalities (7.13) hold, then by Gershgorin's theorem (Lancaster and Tismenetsky, 1985) all the eigen values of  $\tilde{M}$  have negative real parts, and the theorem follows.

We now show that under certain conditions  $\tilde{E}$  is globally asymptotically stable. We first prove a lemma.

Lemma 7.2.3. The region

$$\Omega_1 \equiv \left\{ (C_r, C, C_a) : 0 \leq C_r \leq \frac{q}{r_0} ; 0 \leq C + C_a \leq \frac{Q}{\delta_m} \right\}$$

where  $\delta_m = \min(\delta_0, \delta_a(1 - \theta))$ , is a region of attraction.

Proof : As before

$$\lim_{t \rightarrow \infty} C_r(t) \leq \frac{q}{r_0}$$

$$\text{and } \dot{C} + \dot{C}_a \leq -\delta_m(C + C_a) + Q$$

Hence  $\lim_{t \rightarrow \infty} (C + C_a) \rightarrow \frac{Q}{\delta_m}$ , proving the lemma.

THEOREM 7.2.4 Let the following inequalities hold,

$$\left( (\alpha + \nu_a) \frac{Q}{\delta_m} + \nu \frac{q}{r_0} \right)^2 < (r_0 + \nu \tilde{C}_a)(\delta_a + \nu_a \tilde{C}_r) \quad (7.14a)$$

$$\alpha^2 Q^2 < \delta_m^2 (r_0 + \nu \tilde{C}_a)(\delta_0 + \alpha \tilde{C}_r) \quad (7.14b)$$

$$(\theta \delta_a + \alpha \tilde{C}_r)^2 < (\delta_a + \nu_a \tilde{C}_r)(\delta_0 + \alpha \tilde{C}_r) \quad (7.14c)$$

then  $\tilde{E}$  is globally asymptotically stable.

PROOF : Consider the following positive definite function about  $\tilde{E}$ ,

$$V(C_r, C, C_a) = \frac{1}{2} (C_r - \tilde{C}_r)^2 + \frac{1}{2} (C - \tilde{C})^2 + \frac{1}{2} (C_a - \tilde{C}_a)^2 \quad (7.15)$$

The derivative of  $V$  with respect to  $t$  along solutions can be

written as,

$$\begin{aligned} \dot{V} = & (C_r - \tilde{C}_r) \left( q - r(C_a)C_r \right) + (C - \tilde{C}) \left( -\delta_0 C - \alpha C C_r + \theta \delta_a C_a + q \right) \\ & + (C_a - \tilde{C}_a) \left( -\delta_a C_a + \alpha C C_r - \nu_a C_r C_a \right) \end{aligned} \quad (7.16)$$

After some algebraic manipulations, it can be written as

$$\begin{aligned} \dot{V} = & - (r_0 + \nu \tilde{C}_a) (C_r - \tilde{C}_r)^2 + \left( (\alpha C - \nu_a C_a) - \nu C_r \right) (C_r - \tilde{C}_r) (C_a - \tilde{C}_a) \\ & - (\delta_0 + \alpha \tilde{C}_r) (C - \tilde{C})^2 - \alpha C (C - \tilde{C}) (C_r - \tilde{C}_r) \\ & - (\delta_a + \nu_a \tilde{C}_r) (C_a - \tilde{C}_a)^2 + (\theta \delta_a + \alpha \tilde{C}_r) (C - \tilde{C}) (C_a - \tilde{C}_a) \end{aligned} \quad (7.17)$$

which can further be written as the sum of three quadratic forms,

$$\begin{aligned} \dot{V} = & -\frac{1}{2} a_{11} (C_r - \tilde{C}_r)^2 + a_{12} (C_r - \tilde{C}_r) (C_a - \tilde{C}_a) - \frac{1}{2} a_{22} (C_a - \tilde{C}_a)^2 \\ & - \frac{1}{2} a_{22} (C_a - \tilde{C}_a)^2 + a_{23} (C - \tilde{C}) (C_a - \tilde{C}_a) - \frac{1}{2} a_{33} (C - \tilde{C})^2 \\ & - \frac{1}{2} a_{33} (C - \tilde{C})^2 + a_{13} (C - \tilde{C}) (C_r - \tilde{C}_r) - \frac{1}{2} a_{11} (C_r - \tilde{C}_r)^2 \end{aligned} \quad (7.18)$$

where  $a_{11} = r_0 + \nu \tilde{C}_a$ ,  $a_{12} = (\alpha C - \nu_a C_a) - \nu C_r$

$a_{22} = (\delta_a + \nu_a \tilde{C}_r)$ ,  $a_{23} = \theta \delta_a + \alpha \tilde{C}_r$

$a_{33} = (\delta_0 + \alpha \tilde{C}_r)$ ,  $a_{13} = -\alpha C$

Thus a sufficient condition for  $\dot{V}$  to be negative definite is that

$$a_{12}^2 - a_{11} a_{22} < 0 \quad (7.19a)$$

$$a_{13}^2 - a_{11} a_{33} < 0 \quad (7.19b)$$

$$a_{23}^2 - a_{22} a_{33} < 0 \quad (7.19c)$$

hold. However (7.14a) implies (7.19a), (7.14b) implies (7.19b) and

(7.14c) implies (7.19c). Hence  $\dot{V}$  is a negative definite and so  $V$  is a Liapunov function with respect to  $\tilde{E}$ , whose domain contains  $\Omega_1$ , proving the theorem.

This theorem shows that provided the inequalities (7.14) hold, the system settles down to a steady state and as the removal rate coefficient  $\nu_a$  increases the concentration of the pollutant in the atmosphere decreases and it may even tend to zero if  $\nu_a$  is very large.

### 7.3a ANALYSIS WITH SECONDARY POLLUTANT

Now we will analyze the model (7.1), (7.2), (7.3), and (7.4) considering the formation of secondary pollutant in the atmosphere as well.

#### 7.3.1 CASE I $Q(t) \equiv 0$ (Instantaneous Source)

In this case our model (7.1 - 7.4) has only one non-negative equilibria in the  $C_r - C - C_p - C_a$  space, namely,  $E_1(\frac{q}{r}, 0, 0, 0)$ . The variational matrix corresponding to  $E_1$  is given by  $M_1$  as follows,

$$M_1 = \begin{bmatrix} -r_0 & 0 & 0 & -\nu \frac{q}{r_0} \\ 0 & -(\delta_0 + \lambda + \alpha \frac{q}{r_0}) & 0 & \theta \delta_a \\ 0 & \lambda & -(\delta_1 + \alpha_1 \frac{q}{r_0}) & \theta_1 \delta_a \\ 0 & \alpha \frac{q}{r_0} & \alpha_1 \frac{q}{r_0} & -(\delta_a + \nu_a \frac{q}{r_0}) \end{bmatrix}$$

To determine the local and global stability behavior, we propose the following theorems.

**THEOREM 7.3.1** If the following inequalities hold,

$$(\theta + \theta_1) \delta_a < \delta_a + (\nu_a - \nu) \frac{q}{r_0} \quad (7.20)$$

then  $E_1$  is locally asymptotically stable.

PROOF : The proof follows similarly as in Theorem 7.2.2.

THEOREM 7.3.2 If  $C_r(0) > 0$ , then  $E_1$  is globally asymptotically stable with respect to the non-negative octant.

PROOF : First we note, as before

$$\begin{aligned}\frac{dC_r}{dt} &= \dot{C}_r = q - r(C_a)C_r \\ &\leq q - r_0 C_r\end{aligned}$$

$$\text{Hence } \lim_{t \rightarrow \infty} C_r(t) \leq \frac{q}{r_0}$$

Now consider

$$\begin{aligned}\dot{C} + \dot{C}_p + \dot{C}_a &= - \left( \delta_0 C + \delta_1 C_p + \delta_a C_a (1 - \theta - \theta_1) + \nu_a C_r C_a \right) \\ &\leq - \left( \delta_0 C + \delta_1 C_p + \delta_a C_a (1 - \theta - \theta_1) \right) \\ &\leq - \delta_n (C + C_p + C_a)\end{aligned}$$

$$\text{where } \delta_n = \min(\delta_0, \delta_1, \delta_a(1 - \theta - \theta_1))$$

$$\text{Thus } C(t) + C_p(t) + C_a(t) \leq (C(0) + C_p(0) + C_a(0)) e^{-\delta_n t},$$

hence the system is dissipative. From the above it follows that

$$\lim_{t \rightarrow \infty} C(t) = \lim_{t \rightarrow \infty} C_p(t) = \lim_{t \rightarrow \infty} C_a(t) = 0, \text{ Hence in the limit } C_r(t)$$

is given by the solution of  $\dot{C}_r(t) = q - r_0 C_r$ , since  $C_r(0) > 0$ , and the theorem follows.

This theorem implies that in the case of instantaneous introduction of primary pollutant in the atmosphere and consequential formation of secondary pollutant, the process of precipitation scavenging will remove both primary and secondary pollutants from the atmosphere completely.



### 7.3.2 CASE II $Q(t) \equiv Q > 0$ (Constant Source)

In this case our model again has only one non-negative equilibria  $E^*(C_r^*, C^*, C_p^*, C_a^*)$  in the  $C_r$ - $C$ - $C_p$ - $C_a$  space.

To prove that  $E^*$  exist, we show that the system of algebraic equations,

$$q - r(C_a^*)C_r^* = 0 \quad (7.21)$$

$$-(\delta_0 + \lambda)C^* - \alpha C^*C_r^* + \theta\delta_a C_a^* + Q = 0 \quad (7.22)$$

$$-\delta_1 C_p^* + \lambda C^* - \alpha_1 C_p^*C_r^* + \theta_1\delta_a C_a^* = 0 \quad (7.23)$$

$$-\delta_a C_a^* + \alpha C^*C_r^* + \alpha_1 C_p^*C_r^* - \nu_a C_r^*C_a^* = 0 \quad (7.24)$$

has a positive solution.

$$\text{Equation (7.21) gives, } C_r^* = \frac{q}{r(C_a^*)}, \quad (7.25)$$

substituting  $C_r^*$  in equation (7.22) and (7.24), we get

$$C^* = \frac{Q + \theta\delta_a C_a^*}{\lambda + \delta_0 + \alpha \frac{q}{r(C_a^*)}} \quad (7.26)$$

$$C^* = \frac{C_a^* \left( \delta_a r(C_a^*) + q\nu_a \right)}{\alpha q} - \frac{\alpha_1}{\alpha} C_p^* \quad (7.27)$$

where  $C_p^*$ , is given by, after using  $C_r^*$  in equation (7.23)

$$C_p^* = \frac{\theta_1\delta_a C_a^* + \lambda f_1}{\delta_1 + \alpha_1 \frac{q}{r(C_a^*)}} \quad (7.28)$$

$$\text{and } f_1 = \frac{Q + \theta\delta_a C_a^*}{\lambda + \delta_0 + \alpha \frac{q}{r(C_a^*)}}$$

From equation (7.28) it is noted that  $C_p^*$  increases as  $C_a^*$  increases. And

$$C_p^* \rightarrow \frac{Q \lambda \left( \delta_1 + \alpha_1 \frac{q}{r_0} \right)}{\lambda + \delta_0 + \alpha \frac{q}{r_0}} = C_{p1}^* \text{ (say) } > 0, \text{ as } C_a^* \rightarrow 0$$

We also note from equation (7.28) that when  $\lambda$ ,  $\alpha_1$ , and  $\theta_1$  are zero,  $C_p^*$  is zero. Further we note from equation (7.27) that  $C^*$  varies with  $\nu_a$  through the first term only and thus the equilibrium point, if it exists, will have similar behavior with respect to  $\nu_a$  as in the case of (7.2.2) without secondary pollutant.

Now we will show that the two isoclines (7.26) & (7.27) intersect in the interior of  $C^*-C_a^*$  plane.

From equation (7.26) it is seen that  $C^*$  increases as  $C_a^*$  increases

$$\text{and } C^* \rightarrow \frac{Q}{\lambda + \delta_0 + \alpha \frac{q}{r_0}} = C_1^* \text{ (say) } > 0 \text{ as } C_a^* \rightarrow 0$$

From equation (7.27) it is seen that as  $C_a^* \rightarrow 0$ ,  $C^* \rightarrow -\frac{\alpha_1}{\alpha} C_{p1}^*$  since  $C_p^* \rightarrow C_{p1}^*$  as  $C_a^* \rightarrow 0$ . We also note from equation (7.27) that to lie  $C^*$  in +ve quadrant, the condition,

$$\frac{C_a^* \left( \delta_a r(C_a^*) + q \nu_a \right)}{q} > \alpha_1 C_p^*, \text{ must hold.}$$

Hence two isoclines would intersect as shown in Figure 7.2 and give positive equilibrium provided, the line segment  $R_2 R_3 < R_1 R_3$  where the coordinate of  $R_3$  is  $(Q/\delta_n, 0)$  and this condition can be written by the equations (7.26) & (7.27) as,

$$\alpha f_1^* + \alpha_1 \frac{(\theta_1 \delta_a + \lambda f_1^*) (r_0 \delta_n + \nu Q)}{\delta_1 (r_0 \delta_n + \nu Q) + \alpha_1 q \delta_n} < \frac{\delta_a (r_0 \delta_n + \nu Q) + q \nu_a \delta_n}{q \delta_n} \quad (7.29)$$

$$\text{where } f_1^* = \frac{(\delta_n + \theta \delta_a)(r_0 \delta_n + \nu Q)}{\{(\lambda + \delta_0)(r_0 \delta_n + \nu Q) + \alpha_1 q \delta_n\}}$$

and  $\delta_n = \min\{\delta_0, \delta_1, \delta_a(1 - \theta - \theta_1)\}$ , see lemma 7.3.4.

From Figure 7.2 it is noted that as  $\nu_a$  increases the equilibrium level of  $C^*$  and  $C_a^*$  decreases as in Figure 7.1 and thus the equilibrium level of  $C_p^*$  decreases since  $C_a^*$  decreases (see Eq. 7.28) and hence both primary and secondary pollutants will be removed and may even tend to zero if  $\nu_a$  is very large.

Now the variational matrix corresponding to  $E^*$  is given by  $M^*$  as follows,

$$M^* = \begin{bmatrix} -r(C_a^*) & 0 & 0 & -\nu C_r^* \\ -\alpha C^* & -(\delta_0 + \lambda + \alpha C_r^*) & 0 & \theta \delta_a \\ -\alpha_1 C_p^* & \lambda & -(\delta_1 + \alpha_1 C_r^*) & \theta_1 \delta_a \\ \alpha C^* + \alpha_1 C_p^* - \nu_a C_a^* & \alpha C_r^* & \alpha_1 C_r^* & -(\delta_a + \nu_a C_r^*) \end{bmatrix}$$

**THEOREM 7.3.3** Let the following inequalities hold

$$\begin{aligned} 2(\alpha C^* + \alpha_1 C_p^*) &< r(C_a^*) + \nu_a C_a^* \\ (\nu - \nu_a) C_r^* &< \delta_a(1 - \theta - \theta_1) \end{aligned} \tag{7.30}$$

Then  $E^*$  is locally asymptotically stable.

**PROOF :** The proof follows similarly as in Theorem 7.2.2.

We now show that under certain conditions  $E^*$  is globally asymptotically stable. We first prove a lemma.

Lemma 7.3.4. The region

$$\Omega_2 \equiv \left\{ (C_r, C, C_p, C_a) : 0 \leq C_r \leq \frac{q}{r_0} ; 0 \leq C + C_p + C_a \leq \frac{Q}{\delta_n} \right\}$$

where  $\delta_n = \min (\delta_0, \delta_1, \delta_a(1 - \theta - \theta_1))$ , is a region of attraction.

Proof : As before

$$\lim_{t \rightarrow \infty} C_r(t) \leq \frac{q}{r_0}$$

$$\text{and } \dot{C} + \dot{C}_p + \dot{C}_a \leq -\delta_n(C + C_p + C_a) + Q$$

Hence  $\lim_{t \rightarrow \infty} (C + C_p + C_a) \rightarrow \frac{Q}{\delta_n}$ , proving the lemma.

THEOREM 7.3.5 Let the following inequalities hold,

$$\left( (\alpha + \alpha_1 + \nu_a) \frac{Q}{\delta_n} + \nu \frac{q}{r_0} \right)^2 < \frac{4}{9} (r_0 + \nu C_a^*) (\delta_a + \nu C_r^*) \quad (7.31a)$$

$$\alpha^2 Q^2 < \frac{4}{9} \delta_n^2 (r_0 + \nu C_a^*) (\delta_0 + \lambda + \alpha C_r^*) \quad (7.31b)$$

$$(\theta \delta_a + \alpha C_r^*)^2 < \frac{4}{9} (\delta_a + \nu C_r^*) (\delta_0 + \lambda + \alpha C_r^*) \quad (7.31c)$$

$$(\theta_1 \delta_a + \alpha_1 C_r^*)^2 < \frac{4}{9} (\delta_a + \nu C_r^*) (\delta_1 + \alpha_1 C_r^*) \quad (7.31d)$$

$$\alpha_1^2 Q^2 < \frac{4}{9} \delta_n^2 (r_0 + \nu C_a^*) (\delta_1 + \alpha_1 C_r^*) \quad (7.31e)$$

$$\lambda^2 < \frac{4}{9} (\delta_1 + \alpha_1 C_r^*) (\delta_0 + \lambda + \alpha C_r^*) \quad (7.31f)$$

then  $E^*$  is globally asymptotically stable.

PROOF : Consider the following positive definite function about  $E^*$

$$\begin{aligned} V(C_r, C, C_p, C_a) &= \frac{1}{2} (C_r - C_r^*)^2 + \frac{1}{2} (C - C^*)^2 + \frac{1}{2} (C_p - C_p^*)^2 \\ &\quad + \frac{1}{2} (C_a - C_a^*)^2 \end{aligned} \quad (7.32)$$

The derivative of  $V$  with respect to  $t$  along solutions can be written as,

$$\begin{aligned}
\dot{V} = & (C_r - C_r^*) \left( q - r(C_a)C_r \right) + (C - C^*) \left( -(\delta_0 + \lambda)C - \alpha C C_r \right. \\
& + \theta \delta_a C_a + Q \left. \right) + (C_p - C_p^*) \left( -\delta_1 C_p + \lambda C - \alpha_1 C_p C_r + \theta_1 \delta_a C_a \right) \\
& + (C_a - C_a^*) \left( -\delta_a C_a + \alpha C C_r + \alpha_1 C_p C_r - \nu_a C_r C_a \right) \quad (7.33)
\end{aligned}$$

After some algebraic manipulations, it can be written as,

$$\begin{aligned}
\dot{V} = & - (r_0 + \nu C_a^*)(C_r - C_r^*)^2 + \left( (\alpha C + \alpha_1 C_p - \nu_a C_a) - \nu C_r \right) (C_r - C_r^*)(C_a - C_a^*) \\
& - (\delta_0 + \lambda + \alpha C_r^*)(C - C^*)^2 - \alpha C (C - C^*)(C_r - C_r^*) \\
& - (\delta_1 + \alpha_1 C_r^*)(C_p - C_p^*)^2 + (\theta \delta_a + \alpha C_r^*)(C - C^*)(C_a - C_a^*) \\
& - (\delta_a + \nu_a C_r^*)(C_a - C_a^*)^2 + (\theta_1 \delta_a + \alpha_1 C_r^*)(C_a - C_a^*)(C_p - C_p^*) \\
& + \lambda (C - C^*)(C_p - C_p^*) - \alpha_1 C_p (C_r - C_r^*)(C_p - C_p^*) .
\end{aligned}$$

which can further be written as the sum of the quadratics as

$$\begin{aligned}
\dot{V} = & -\frac{1}{2} a_{11} (C_r - C_r^*)^2 + a_{12} (C_r - C_r^*)(C_a - C_a^*) - \frac{1}{2} a_{22} (C_a - C_a^*)^2 \\
& - \frac{1}{2} a_{11} (C_r - C_r^*)^2 + a_{13} (C_r - C_r^*)(C - C^*) - \frac{1}{2} a_{33} (C - C^*)^2 \\
& - \frac{1}{2} a_{22} (C_a - C_a^*)^2 + a_{23} (C_a - C_a^*)(C - C^*) - \frac{1}{2} a_{33} (C - C^*)^2 \\
& - \frac{1}{2} a_{22} (C_a - C_a^*)^2 + a_{24} (C_a - C_a^*)(C_p - C_p^*) - \frac{1}{2} a_{44} (C_p - C_p^*)^2 \\
& - \frac{1}{2} a_{11} (C_r - C_r^*)^2 + a_{14} (C_r - C_r^*)(C_p - C_p^*) - \frac{1}{2} a_{44} (C_p - C_p^*)^2 \\
& - \frac{1}{2} a_{33} (C - C^*)^2 + a_{34} (C - C^*)(C_p - C_p^*) - \frac{1}{2} a_{44} (C_p - C_p^*)^2
\end{aligned}$$

$$\begin{aligned}
\text{where } a_{11} &= \frac{2}{3} (r_0 + \nu C_a^*), & a_{12} &= (\alpha C + \alpha_1 C_p - \nu_a C_a) - \nu C_r \\
a_{22} &= \frac{2}{3} (\delta_a + \nu_a C_r^*), & a_{13} &= -\alpha C \\
a_{33} &= \frac{2}{3} (\delta_0 + \lambda + \alpha C_r^*), & a_{23} &= \theta \delta_a + \alpha C_r^* \\
a_{44} &= \frac{2}{3} (\delta_1 + \alpha_1 C_r^*), & a_{24} &= \theta_1 \delta_a + \alpha_1 C_r^* \\
a_{14} &= -\alpha_1 C_p, & a_{34} &= \lambda
\end{aligned}$$

Thus a sufficient condition for  $\dot{V}$  to be negative definite is that

$$a_{12}^2 - a_{11} a_{22} < 0 \quad (7.34a)$$

$$a_{13}^2 - a_{11} a_{33} < 0 \quad (7.34b)$$

$$a_{23}^2 - a_{22} a_{33} < 0 \quad (7.34c)$$

$$a_{24}^2 - a_{22} a_{44} < 0 \quad (7.34d)$$

$$a_{14}^2 - a_{11} a_{44} < 0 \quad (7.34e)$$

$$a_{34}^2 - a_{33} a_{44} < 0 \quad (7.34f)$$

hold. However (7.31a - 7.31f) implies (7.34a - 7.34f) respectively. Hence  $\dot{V}$  is a negative definite and so  $V$  is a Liapunov function with respect to  $E^*$ , containing the domain  $\Omega_2$ , proving the theorem.

This theorem shows that if there is constant emission of the pollutant then even in that case both the pollutants can be removed from the atmosphere and this rate of removal would depend upon the rate of introduction of the pollutant and other parameters.

#### 7.4 CONCLUSION

We have proposed a nonlinear ecological type model for removal mechanism of both primary and secondary air pollutants in the atmosphere by the precipitation scavenging. Using stability analysis it has been shown that when the pollutant is emitted in the atmosphere by an instantaneous source (single introduction of the pollutant in the atmosphere), the pollutants from the atmosphere would be completely removed by the precipitation scavenging. When the pollutant is emitted at a constant rate in the atmosphere it is found that the pollutants may be removed from the atmosphere completely but it would depend upon the rate of emission and removal by precipitation and other processes.

The proposed model and analysis presented here also suggests that to remove the pollutants from the atmosphere, external species may be introduced in the atmosphere which can interact with the pollutant and remove it by some suitable removal processes based upon the physical and chemical properties of the pollutants as well as that of externally introduced species.

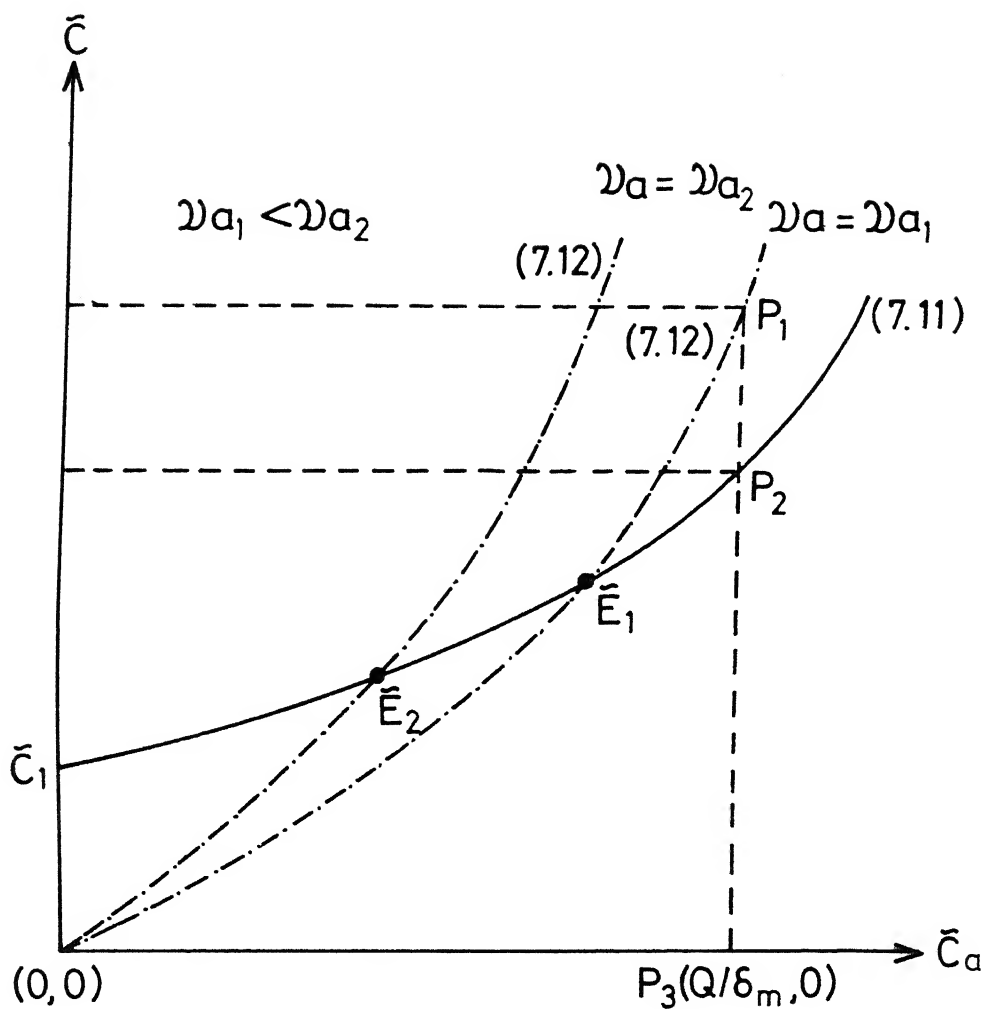


FIG.7.1 INTERSECTION OF TWO ISOCLINES (7.11) AND (7.12) TO DETERMINE  $\tilde{E}$  .



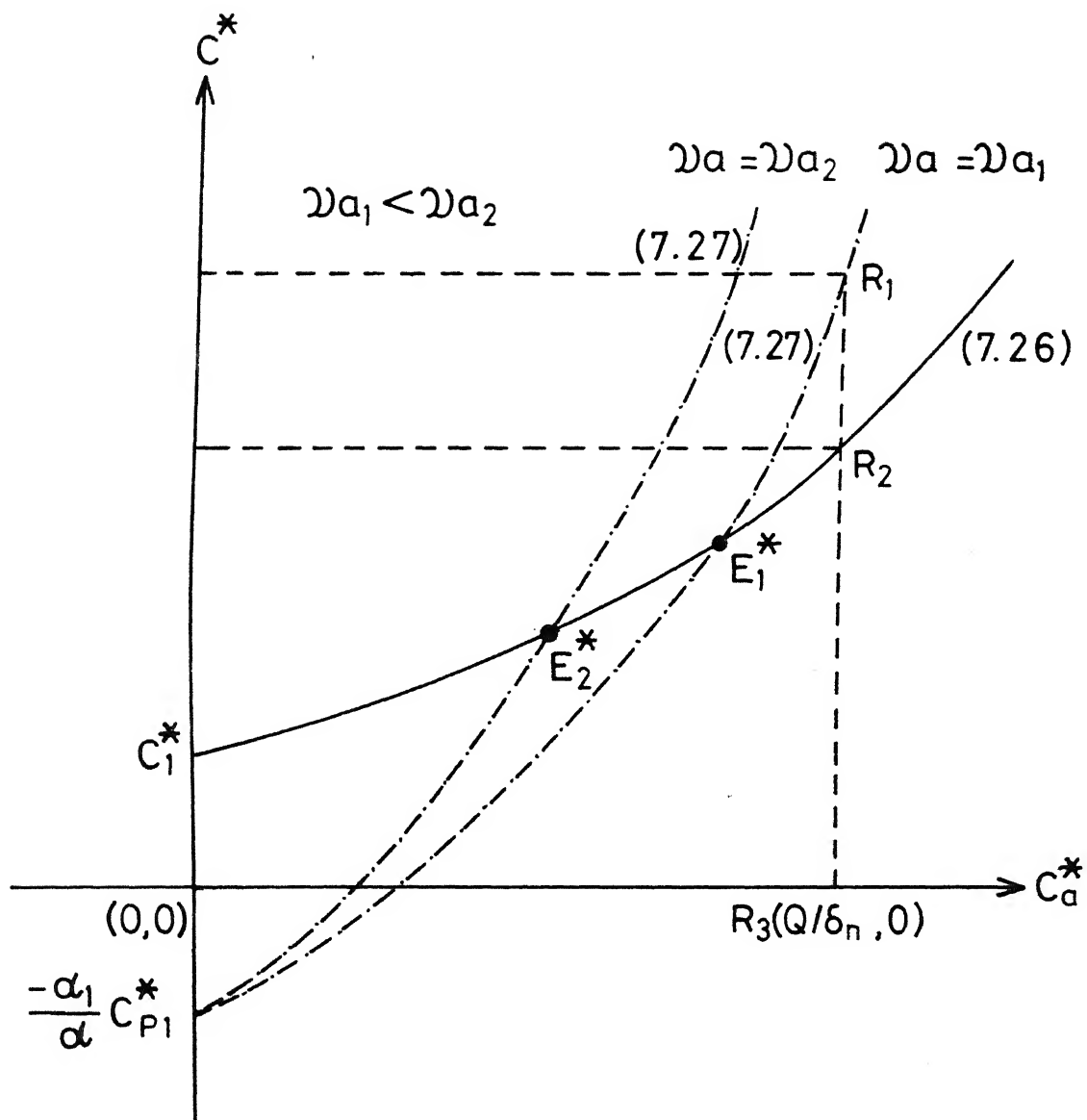


FIG.7.2 INTERSECTION OF TWO ISOCLINES (7.26) AND (7.27) TO DETERMINE  $E^*$ .

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